

AM-95-599

Derivation and identification of nonstandard serpentine polytypes

Sturges W. Bailey, Jillian F. Banfield

For deposit: Table 3

American Mineralogist, 80, 11-12, 1104-1115.

FOR MSA DEPOSIT

Atomic coordinates of 14 regular-stacking serpentine structural models

from: "Derivation and identification of non-standard serpentine polytypes"

by Sturges W. Bailey and Jillian F. Banfield

TITL	2tc102modell1 in C1						
CELL	0.71073	5.323	9.432	14.567	102.16	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O MG SI						
UNIT	36	12	8				
O1	1	10.5000	.0000	10.0000	Two-layer, alpha = 102		
O2	1	10.2500	.2500	10.0000			
O3	1	10.2500	.7500	10.0000	2Tc (= 6R2), model 1		
Si1	3	.5000	.1802	.0414	0, -b/3		
Si2	3	.5000	.8468	.0414			
O4	1	.0000	.0513	.1576	I, II		
O5	1	.5000	.2180	.1576			
O6	1	.5000	.8846	.1576	C1		
Mg1	2	.3333	.0759	.2332			
Mg2	2	.3333	.4092	.2332			
Mg3	2	.3333	.7426	.2332			
O7	1	.6667	.0987	.3034			
O8	1	.6667	.4320	.3034			
O9	1	.6667	.7654	.3034			
O10	1	.5000	.1627	.5000			
O11	1	.2500	.4127	.5000			
O12	1	.2500	.9127	.5000			
Si3	3	.5000	.3428	.5414			
Si4	3	.5000	.0094	.5414			
O13	1	.0000	.2139	.6576			
O14	1	.5000	.3806	.6576			
O15	1	.5000	.0472	.6576			
Mg4	2	.6667	.2385	.7332			
Mg5	2	.6667	.5718	.7332			
Mg6	2	.6667	.9052	.7332			
O16	1	.3333	.2614	.8034			
O17	1	.3333	.5947	.8034			
O18	1	.3333	.9281	.8034			

TTITL 3tc98model2 in C1

CELL	0.71073	5.323	9.214	21.599	98.18	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O	Mg	SI				
UNIT	54	18	12				
O1	1	10.0000	.5000	10.0000			Three-layer, alpha = 98
O2	1	10.2500	.2500	10.0000			
O3	1	10.7500	.2500	10.0000			Model 2
Si1	3	.0000	.3425	.0276			
Si2	3	.0000	.6759	.0276			0,+b/3,+b/3
O4	1	.0000	.0351	.1051			
O5	1	.0000	.3684	.1051			I,I,II
O6	1	.0000	.7018	.1051			
Mg1	2	.3333	.0519	.1555			C1
Mg2	2	.3333	.3852	.1555			
Mg3	2	.3333	.7186	.1555			
O7	1	.6667	.0676	.2023			
O8	1	.6667	.4009	.2023			
O9	1	.6667	.7343	.2023			
O10	1	.0000	.6113	.3333			
O11	1	.2500	.3613	.3333			
O12	1	.2500	.8613	.3333			
Si3	3	.0000	.4538	.3609			
Si4	3	.0000	.7872	.3609			
O13	1	.0000	.1464	.4384			
O14	1	.0000	.4797	.4384			
O15	1	.0000	.8131	.4384			
Mg4	2	.3333	.1632	.4888			
Mg5	2	.3333	.4965	.4888			
Mg6	2	.3333	.8299	.4888			
O16	1	.6667	.1788	.5356			
O17	1	.6667	.5121	.5356			
O18	1	.6667	.8455	.5356			
O19	1	.0000	.0559	.6667			
O20	1	.2500	.3059	.6667			
O21	1	.7500	.3059	.6667			
Si5	3	.0000	.2318	.6943			
Si6	3	.0000	.8985	.6943			
O22	1	.0000	.5910	.7718			
O23	1	.0000	.2577	.7718			
O24	1	.0000	.9244	.7718			
Mg7	2	.6667	.2745	.8222			
Mg8	2	.6667	.6078	.8222			
Mg9	2	.6667	.9412	.8222			
O25	1	.3333	.2901	.8690			
O26	1	.3333	.6234	.8690			
O27	1	.3333	.9568	.8690			

TITL	3tc98model3 in C1						
CELL	0.71073	5.323	9.214	21.599	98.18	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O MG SI						
UNIT	54	18	12				
O1	1	10.5000	.0000	10.0000	Three-layer, alpha = 98		
O2	1	10.2500	.2500	10.0000			
O3	1	10.2500	.7500	10.0000	Model 3		
Si1	3	.5000	.1759	.0276			
Si2	3	.5000	.8425	.0276	-b/3, -b/3, +b/3		
O4	1	.0000	.0351	.1051			
O5	1	.5000	.2018	.1051	I, I, II		
O6	1	.5000	.8684	.1051			
Mg1	2	.3333	.0519	.1555	C1		
Mg2	2	.3333	.3852	.1555			
Mg3	2	.3333	.7185	.1555			
O7	1	.6667	.0676	.2023			
O8	1	.6667	.4009	.2023			
O9	1	.6667	.7343	.2023			
O10	1	.0000	.2780	.3333			
O11	1	.2500	.0280	.3333			
O12	1	.7500	.0280	.3333			
Si3	3	.0000	.1205	.3609			
Si4	3	.0000	.4538	.3609			
O13	1	.0000	.8128	.4384			
O14	1	.0000	.1464	.4384			
O15	1	.0000	.4797	.4384			
Mg4	2	.3333	.1632	.4888			
Mg5	2	.3333	.4965	.4888			
Mg6	2	.3333	.8299	.4888			
O16	1	.6667	.1788	.5356			
O17	1	.6667	.5121	.5356			
O18	1	.6667	.8455	.5356			
O19	1	.2500	.3059	.6667			
O20	1	.2500	.8059	.6667			
O21	1	.5000	.5559	.6667			
Si5	3	.0000	.2318	.6943			
Si6	3	.0000	.8985	.6943			
O22	1	.0000	.5910	.7718			
O23	1	.0000	.2577	.7718			
O24	1	.0000	.9244	.7718			
Mg7	2	.6667	.2745	.8222			
Mg8	2	.6667	.6078	.8222			
Mg9	2	.6667	.9412	.8222			
O25	1	.3333	.2901	.8690			
O26	1	.3333	.6234	.8690			
O28	1	.3333	.9568	.8690			

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TITL 3tc98model4 in C1
CELL 0.71073 5.323 9.214 21.599 98.18 90.00 90.00
ZERR 2.00 0.001 0.002 0.004 0.03 0.03 0.03
LATT -7
SFAC O MG SI
UNIT 54 18 12
O1 1 10.5000 .0000 10.0000 Three-layer, alpha = 98
O2 1 10.2500 .2500 10.0000
O3 1 10.2500 .7500 10.0000 Model 4
Si1 3 .5000 .1759 .0276
Si2 3 .5000 .8425 .0276 0,0,-b/3
O4 1 .0000 .0351 .1051
O5 1 .5000 .2018 .1051 I,I,II
O6 1 .5000 .8684 .1051
Mg1 2 .3333 .0519 .1555 C1
Mg2 2 .3333 .3852 .1555
Mg3 2 .3333 .7185 .1555
O7 1 .6667 .0676 .2023
O8 1 .6667 .4009 .2023
O9 1 .6667 .7343 .2023
O10 1 .5000 .1113 .3333
O11 1 .2500 .3613 .3333
O12 1 .2500 .8613 .3333
Si3 3 .5000 .2872 .3609
Si4 3 .5000 .9538 .3609
O13 1 .0000 .1464 .4384
O14 1 .5000 .3131 .4384
O15 1 .5000 .9797 .4384
Mg4 2 .3333 .1632 .4888
Mg5 2 .3333 .4965 .4888
Mg6 2 .3333 .8299 .4888
O16 1 .6667 .1788 .5356
O17 1 .6667 .5121 .5356
O18 1 .6667 .8455 .5356
O19 1 .0000 .3893 .6667
O20 1 .2500 .1393 .6667
O21 1 .7500 .1393 .6667
Si5 3 .0000 .2318 .6943
Si6 3 .0000 .5651 .6943
O22 1 .0000 .9244 .7718
O23 1 .0000 .2577 .7718
O24 1 .0000 .5910 .7718
Mg7 2 .1667 .4412 .8222
Mg8 2 .1667 .7745 .8222
Mg9 2 .1667 .1078 .8222
O25 1 .3333 .2901 .8690
O26 1 .3333 .6234 .8690
O28 1 .3333 .9568 .8690

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TITL	3m90model5 in C1						
CELL	0.71073	5.323	9.220	21.360	90.00	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O MG SI						
UNIT	54	18	12				
O1	1	10.0000	.5000	10.0000	Three-layer, alpha = 90		
O2	1	10.2500	.2500	10.0000			
O3	1	10.7500	.2500	10.0000	Model 5		
Si1	3	.0000	.3333	.0276			
Si2	3	.0000	.6667	.0276	0, -b/3, +b/3		
O4	1	.0000	.0000	.1051			
O5	1	.0000	.3333	.1051	I, I, II		
O6	1	.0000	.6667	.1051			
Mg1	2	.3333	.0000	.1555	C1		
Mg2	2	.3333	.3333	.1555			
Mg3	2	.3333	.6667	.1555			
O7	1	.6667	.0000	.2023			
O8	1	.6667	.3333	.2023			
O9	1	.6667	.6667	.2023			
O10	1	.0000	.5000	.3333			
O11	1	.2500	.2500	.3333			
O12	1	.2500	.7500	.3333			
Si3	3	.0000	.3333	.3609			
Si4	3	.0000	.6667	.3609			
O13	1	.0000	.0000	.4384			
O14	1	.0000	.3333	.4384			
O15	1	.0000	.6667	.4384			
Mg4	2	.3333	.0000	.4888			
Mg5	2	.3333	.3333	.4888			
Mg6	2	.3333	.6667	.4888			
O16	1	.6667	.0000	.5356			
O17	1	.6667	.3333	.5356			
O18	1	.6667	.6667	.5356			
O19	1	.0000	.1667	.6667			
O20	1	.2500	.4167	.6667			
O21	1	.7500	.4167	.6667			
Si5	3	.0000	.0000	.6943			
Si6	3	.0000	.3333	.6943			
O22	1	.0000	.6667	.7718			
O23	1	.0000	.0000	.7718			
O24	1	.0000	.3333	.7718			
Mg7	2	.6667	.0000	.8222			
Mg8	2	.6667	.3333	.8222			
Mg9	2	.6667	.6667	.8222			
O25	1	.3333	.0000	.8690			
O26	1	.3333	.3333	.8690			
O27	1	.3333	.6667	.8690			

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TITL 4tc96model6 in Cl
CELL 0.71073 5.323 9.268 28.315 96.26 90.00 90.00
ZERR 2.00 0.001 0.002 0.004 0.03 0.03 0.03
LATT -7
SFAC O MG SI
UNIT 72 24 16
O1 1 10.5000 .0000 10.0000 Four-layer, alpha = 96
O2 1 10.2500 .2500 10.0000
O3 1 10.2500 .7500 10.0000 Model 6
Si1 3 .5000 .1736 .0207
Si2 3 .5000 .8402 .0207 0,0,0,-b/3
O4 1 .0000 .0263 .0788
O5 1 .5000 .1930 .0788 I,II,I,II
O6 1 .5000 .8596 .0788
Mg1 2 .3333 .0388 .1166 Cl
Mg2 2 .3333 .3721 .1166
Mg3 2 .3333 .7055 .1166
O7 1 .6667 .0505 .1517
O8 1 .6667 .3838 .1517
O9 1 .6667 .7172 .1517
O10 1 .5000 .0833 .2500
O11 1 .2500 .3333 .2500
O12 1 .2500 .8333 .2500
Si3 3 .5000 .2569 .2707
Si4 3 .5000 .9235 .2707
O13 1 .0000 .1095 .3288
O14 1 .5000 .2762 .3288
O15 1 .5000 .9428 .3288
Mg4 2 .6667 .1221 .3666
Mg5 2 .6667 .4554 .3666
Mg6 2 .6667 .7885 .3666
O16 1 .3333 .1338 .4017
O17 1 .3333 .4671 .4017
O18 1 .3333 .8005 .4017
O19 1 .5000 .1667 .5000
O20 1 .2500 .4167 .5000
O21 1 .2500 .9167 .5000
Si5 3 .5000 .3402 .5207
Si6 3 .5000 .0068 .5207
O22 1 .0000 .1929 .5789
O23 1 .5000 .3596 .5789
O24 1 .5000 .0262 .5789
Mg7 2 .3333 .2054 .6167
Mg8 2 .3333 .5387 .6167
Mg9 2 .3333 .8721 .6167
O25 1 .6667 .2171 .6517
O26 1 .6667 .5504 .6517
O27 1 .6667 .8838 .6517
O28 1 .5000 .2498 .7500
O29 1 .2500 .4998 .7500
O30 1 .2500 .9998 .7500
Si7 3 .0000 .5900 .7707
Si8 3 .0000 .9234 .7707
O31 1 .0000 .2761 .8288
O32 1 .0000 .6094 .8288
O33 1 .0000 .9428 .8288
Mg10 2 .1667 .4554 .8666
Mg11 2 .1667 .7887 .8666
Mg12 2 .1667 .1200 .8666
O34 1 .3333 .3004 .9017
O35 1 .3333 .6337 .9017
O36 1 .3333 .9671 .9017

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TITL 4tc96model7 in C1
CELL 0.71073 5.323 9.268 28.315 96.26 90.00 90.00
ZERR 2.00 0.001 0.002 0.004 0.03 0.03 0.03
LATT -7
SFAC O MG SI
UNIT 72 24 16
O1 1 10.0000 .5000 10.0000 Four-layer, alpha = 96
O2 1 10.2500 .2500 10.0000
O3 1 10.2500 .7500 10.0000 Model 7
Si1 3 .0000 .3402 .0207
Si2 3 .0000 .6736 .0207 +b/3,+b/3,+b/3,-b/3
O4 1 .0000 .0263 .0788
O5 1 .0000 .3596 .0788 I,I,II,II
O6 1 .0000 .6930 .0788
Mg1 2 .3333 .0388 .1166 C1
Mg2 2 .3333 .3721 .1166
Mg3 2 .3333 .7055 .1166
O7 1 .6667 .0505 .1517
O8 1 .6667 .3838 .1517
O9 1 .6667 .7172 .1517
O10 1 .0000 .9166 .2500
O11 1 .2500 .1667 .2500
O12 1 .2500 .6667 .2500
Si3 3 .0000 .0902 .2707
Si4 3 .0000 .7569 .2707
O13 1 .0000 .4428 .3288
O14 1 .0000 .1095 .3288
O15 1 .0000 .7762 .3288
Mg4 2 .3333 .1221 .3666
Mg5 2 .3333 .4543 .3666
Mg6 2 .3333 .7888 .3666
O16 1 .6667 .1338 .4017
O17 1 .6667 .4671 .4017
O18 1 .6667 .8005 .4017
O19 1 .0000 .3333 .5000
O20 1 .2500 .0834 .5000
O21 1 .2500 .5834 .5000
Si5 3 .0000 .1735 .5207
Si6 3 .0000 .5068 .5207
O22 1 .0000 .8596 .5789
O23 1 .0000 .1929 .5789
O24 1 .0000 .5262 .5789
Mg7 2 .6667 .2054 .6167
Mg8 2 .6667 .5387 .6167
Mg9 2 .6667 .8721 .6167
O25 1 .3333 .2171 .6517
O26 1 .3333 .5504 .6517
O27 1 .3333 .8838 .6517
O28 1 .0000 .7498 .7500
O29 1 .2500 .4998 .7500
O30 1 .2500 .9998 .7500
Si7 3 .0000 .5900 .7707
Si8 3 .0000 .9234 .7707
O31 1 .0000 .9428 .8288
O32 1 .0000 .2761 .8288
O33 1 .0000 .6094 .8288
Mg10 2 .6667 .2887 .8666
Mg11 2 .6667 .6220 .8666
Mg12 2 .6667 .9554 .8666
O34 1 .3333 .3004 .9017
O35 1 .3333 .6337 .9017
O36 1 .3333 .9671 .9017

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TITL	4tc96model8 in C1						
CELL	0.71073	5.323	9.268	28.315	96.26	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O MG SI						
UNIT	72	24	16				
O1	1	10.5000	.0000	10.0000	Four-layer, alpha = 96		
O2	1	10.2500	.2500	10.0000			
O3	1	10.2500	.7500	10.0000	Model 8		
Si1	3	.5000	.1736	.0207			
Si2	3	.5000	.8402	.0207	0, -b/3, -b/3, +b/3		
O4	1	.0000	.0263	.0788			
O5	1	.5000	.1930	.0788	I, I, I, II		
O6	1	.5000	.8596	.0788			
Mg1	2	.3333	.0388	.1166	C1		
Mg2	2	.3333	.3721	.1166			
Mg3	2	.3333	.7055	.1166			
O7	1	.6667	.0505	.1517			
O8	1	.6667	.3838	.1517			
O9	1	.6667	.7172	.1517			
O10	1	.5000	.0833	.2500			
O11	1	.2500	.3333	.2500			
O12	1	.2500	.8333	.2500			
Si3	3	.5000	.2569	.2707			
Si4	3	.5000	.9235	.2707			
O13	1	.0000	.1095	.3288			
O14	1	.5000	.2762	.3288			
O15	1	.5000	.9428	.3288			
Mg4	2	.3333	.1221	.3666			
Mg5	2	.3333	.4554	.3666			
Mg6	2	.3333	.7885	.3666			
O16	1	.6667	.1338	.4017			
O17	1	.6667	.4671	.4017			
O18	1	.6667	.8005	.4017			
O19	1	.0000	.3333	.5000			
O20	1	.2500	.0833	.5000			
O21	1	.7500	.0833	.5000			
Si5	3	.0000	.1735	.5207			
Si6	3	.0000	.5068	.5207			
O22	1	.0000	.8596	.5789			
O23	1	.0000	.1929	.5789			
O24	1	.0000	.5262	.5789			
Mg7	2	.3333	.2054	.6167			
Mg8	2	.3333	.5387	.6167			
Mg9	2	.3333	.8721	.6167			
O25	1	.6667	.2171	.6517			
O26	1	.6667	.5504	.6517			
O27	1	.6667	.8838	.6517			
O28	1	.0000	.0831	.7500			
O29	1	.2500	.3331	.7500			
O30	1	.7500	.3331	.7500			
Si7	3	.0000	.2567	.7707			
Si8	3	.0000	.9234	.7707			
O31	1	.0000	.6094	.8288			
O32	1	.0000	.2761	.8288			
O33	1	.0000	.9428	.8288			
Mg10	2	.6667	.2887	.8666			
Mg11	2	.6667	.6220	.8666			
Mg12	2	.6667	.9554	.8666			
O34	1	.3333	.3004	.9017			
O35	1	.3333	.6337	.9017			
O36	1	.3333	.9671	.9017			

TITL	4tc96model9 in C1						
CELL	0.71073	5.323	9.268	28.315	96.26	90.00	90.00
ZERR	2.00	0.001	0.002	0.004	0.03	0.03	0.03
LATT	-7						
SFAC	O MG SI						
UNIT	72	24	16				
O1	1	10.5000	.0000	10.0000	Four-layer, alpha = 96		
O2	1	10.2500	.2500	10.0000			
O3	1	10.2500	.7500	10.0000	Model 9		
Si1	3	.5000	.1736	.0207			
Si2	3	.5000	.8402	.0207	0, -b/3, +b/3, -b/3		
O4	1	.0000	.0263	.0788			
O5	1	.5000	.1930	.0788	I, I, I, II		
O6	1	.5000	.8596	.0788			
Mg1	2	.3333	.0388	.1166	C1		
Mg2	2	.3333	.3721	.1166			
Mg3	2	.3333	.7055	.1166			
O7	1	.6667	.0505	.1517			
O8	1	.6667	.3838	.1517			
O9	1	.6667	.7172	.1517			
O10	1	.5000	.0833	.2500			
O11	1	.2500	.3333	.2500			
O12	1	.2500	.8333	.2500			
Si3	3	.5000	.2569	.2707			
Si4	3	.5000	.9235	.2707			
O13	1	.0000	.1095	.3288			
O14	1	.5000	.2762	.3288			
O15	1	.5000	.9428	.3288			
Mg4	2	.3333	.1221	.3666			
Mg5	2	.3333	.4554	.3666			
Mg6	2	.3333	.7885	.3666			
O16	1	.6667	.1338	.4017			
O17	1	.6667	.4671	.4017			
O18	1	.6667	.8005	.4017			
O19	1	.0000	.3333	.5000			
O20	1	.2500	.0833	.5000			
O21	1	.7500	.0833	.5000			
Si5	3	.0000	.1735	.5207			
Si6	3	.0000	.5068	.5207			
O22	1	.0000	.8596	.5789			
O23	1	.0000	.1929	.5789			
O24	1	.0000	.5262	.5789			
Mg7	2	.3333	.2054	.6167			
Mg8	2	.3333	.5387	.6167			
Mg9	2	.3333	.8721	.6167			
O25	1	.6667	.2171	.6517			
O26	1	.6667	.5504	.6517			
O27	1	.6667	.8838	.6517			
O28	1	.0000	.7498	.7500			
O29	1	.2500	.4998	.7500			
O30	1	.2500	.9998	.7500			
Si7	3	.0000	.5900	.7707			
Si8	3	.0000	.9234	.7707			
O31	1	.0000	.6094	.8288			
O32	1	.0000	.2761	.8288			
O33	1	.0000	.9428	.8288			
Mg10	2	.6667	.2887	.8666			
Mg11	2	.6667	.6220	.8666			
Mg12	2	.6667	.9554	.8666			
O34	1	.3333	.3004	.9017			
O35	1	.3333	.6337	.9017			
O36	1	.3333	.9671	.9017			

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TITL 4tc96modell10 as C1
CELL 0.71073 5.323 9.268 28.315 96.26 90.00 90.00
ZERR 2.00 0.001 0.002 0.004 0.03 0.03 0.03
LATT -7
SFAC O MG SI
UNIT 72 24 16
O1 1 10.5000 .0000 10.0000 Four-layer, alpha = 96
O2 1 10.2500 .2500 10.0000
O3 1 10.2500 .7500 10.0000 Model 10
Si1 3 .5000 .1736 .0207
Si2 3 .5000 .8402 .0207 0,0,+b/3,+b/3
O4 1 .0000 .0263 .0788
O5 1 .5000 .1930 .0788 I,I,I,II
O6 1 .5000 .8596 .0788
Mg1 2 .3333 .0388 .1166 C1
Mg2 2 .3333 .3721 .1166
Mg3 2 .3333 .7055 .1166
O7 1 .6667 .0505 .1517
O8 1 .6667 .3838 .1517
O9 1 .6667 .7172 .1517
O10 1 .5000 .0833 .2500
O11 1 .2500 .3333 .2500
O12 1 .2500 .8333 .2500
Si3 3 .5000 .2569 .2707
Si4 3 .5000 .9235 .2707
O13 1 .0000 .1095 .3288
O14 1 .5000 .2762 .3288
O15 1 .5000 .9428 .3288
Mg4 2 .3333 .1221 .3666
Mg5 2 .3333 .4554 .3666
Mg6 2 .3333 .7885 .3666
O16 1 .6667 .1338 .4017
O17 1 .6667 .4671 .4017
O18 1 .6667 .8005 .4017
O19 1 .5000 .1667 .5000
O20 1 .2500 .4167 .5000
O21 1 .2500 .9167 .5000
Si5 3 .5000 .3402 .5207
Si6 3 .5000 .0068 .5207
O22 1 .0000 .1929 .5789
O23 1 .5000 .3596 .5789
O24 1 .5000 .0262 .5789
Mg7 2 .3333 .2054 .6167
Mg8 2 .3333 .5387 .6167
Mg9 2 .3333 .8721 .6167
O25 1 .6667 .2171 .6517
O26 1 .6667 .5504 .6517
O27 1 .6667 .8838 .6517
O28 1 .2500 .3331 .7500
O29 1 .7500 .3331 .7500
O30 1 .5000 .5831 .7500
Si7 3 .0000 .2567 .7707
Si8 3 .0000 .9234 .7707
O31 1 .0000 .6094 .8288
O32 1 .0000 .2761 .8288
O33 1 .0000 .9428 .8288
Mg10 2 .6667 .2887 .8666
Mg11 2 .6667 .6220 .8666
Mg12 2 .6667 .9554 .8666
O34 1 .3333 .3004 .9017
O35 1 .3333 .6337 .9017
O36 1 .3333 .9671 .9017

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TITL 4m90modell11 in C1  
 CELL 0.71073 5.314 9.204 28.428 90.00 90.00 90.00  
 ZERR 2.00 0.001 0.002 0.004 0.00 0.00 0.00  
 LATT -7  
 SFAC O MG SI  
 UNIT 72 24 16

O1	1	10.2500	.0833	10.0000
O2	1	10.0000	.8333	10.0000
O3	1	10.7500	.0833	10.0000
Si1	3	.0000	.0000	.0207
Si2	3	.0000	.6667	.0207
O4	1	.0000	.3333	.0788
O5	1	.0000	.0000	.0788
O6	1	.0000	.6667	.0788
Mg1	2	.3333	.0000	.1166
Mg2	2	.3333	.3333	.1166
Mg3	2	.3333	.6667	.1166
O7	1	.6667	.0000	.1517
O8	1	.6667	.3333	.1517
O9	1	.6667	.6667	.1517
O10	1	.5000	.0000	.2500
O11	1	.2500	.2500	.2500
O12	1	.7500	.2500	.2500
Si3	3	.0000	.3333	.2707
Si4	3	.0000	.6667	.2707
O13	1	.0000	.0000	.3288
O14	1	.0000	.3333	.3288
O15	1	.0000	.6667	.3288
Mg4	2	.6667	.0000	.3666
Mg5	2	.6667	.3333	.3666
Mg6	2	.6667	.6667	.3666
O16	1	.3333	.0000	.4017
O17	1	.3333	.3333	.4017
O18	1	.3333	.6667	.4017
O19	1	.0000	.1667	.5000
O20	1	.7500	.9167	.5000
O21	1	.2500	.9167	.5000
Si5	3	.0000	.0000	.5207
Si6	3	.0000	.3333	.5207
O22	1	.0000	.6667	.5789
O23	1	.0000	.0000	.5789
O24	1	.0000	.3333	.5789
Mg7	2	.3333	.0000	.6167
Mg8	2	.3333	.3333	.6167
Mg9	2	.3333	.6667	.6167
O25	1	.6667	.0000	.6517
O26	1	.6667	.3333	.6517
O27	1	.6667	.6667	.6517
O28	1	.5000	.0000	.7500
O29	1	.2500	.7500	.7500
O30	1	.7500	.7500	.7500
Si7	3	.0000	.3333	.7707
Si8	3	.0000	.6667	.7707
O31	1	.0000	.0000	.8288
O32	1	.0000	.3333	.8288
O33	1	.0000	.6667	.8288
Mg10	2	.6667	.0000	.8666
Mg11	2	.6667	.3333	.8666
Mg12	2	.6667	.6667	.8666
O34	1	.3333	.0000	.9017
O35	1	.3333	.3333	.9017
O36	1	.3333	.6667	.9017

Four-layer, alpha = 90

Model 11

-b/3, -b/3, +b/3, +b/3

I, II, I, II

Cc, but only with the  
 the I, II, I, II octahedral  
 cation sequence. Modeled  
 here as C1. X and Y axes  
 are not reversed.

TITL 4m90model12 in C1  
CELL 0.71073 5.314 9.204 28.428 90.00 90.00 90.00  
ZERR 2.00 0.001 0.002 0.004 0.00 0.00 0.00  
LATT -7  
SFAC O MG SI  
UNIT 72 24 16

O1	1	10.6667	.1667	10.0000	Four-layer, alpha = 90
O2	1	.4167	.9167	10.0000	
O3	1	.9167	.9167	.0000	Model 12
Si1	3	.1667	.5000	.0207	
Si2	3	.1667	.8333	.0207	0, -b/3, 0, +b/3
O4	1	.1667	.1667	.0788	
O5	1	.1667	.5000	.0788	I, II, I, II
O6	1	.1667	.8333	.0788	
Mg1	2	.0000	.0000	.1166	Cc with X and Y reversed
Mg2	2	.0000	.3333	.1166	but modeled here as C1
Mg3	2	.0000	.6667	.1166	with usual X and Y. Has
O7	1	.3333	.0000	.1517	Cc symmetry only with the
O8	1	.3333	.3333	.1517	I, II, I, II octahedral cation
O9	1	.3333	.6667	.1517	sequence.
O10	1	.6667	.1667	.2500	
O11	1	.4167	.9167	.2500	
O12	1	.9167	.9167	.2500	
Si3	3	.6667	.0000	.2707	
Si4	3	.6667	.3333	.2707	
O13	1	.6667	.6667	.3288	
O14	1	.6667	.0000	.3288	
O15	1	.6667	.3333	.3288	
Mg4	2	.3333	.0000	.3666	
Mg5	2	.3333	.3333	.3666	
Mg6	2	.3333	.6667	.3666	
O16	1	.0000	.0000	.4017	
O17	1	.0000	.3333	.4017	
O18	1	.0000	.6667	.4017	
O19	1	.6667	.8333	.5000	
O20	1	.9167	.0833	.5000	
O21	1	.4167	.0833	.5000	
Si5	3	.1667	.1667	.5204	
Si6	3	.1667	.5000	.5204	
O22	1	.1667	.8333	.5789	
O23	1	.1667	.1667	.5789	
O24	1	.1667	.5000	.5789	
Mg7	2	.0000	.0000	.6167	
Mg8	2	.0000	.3333	.6167	
Mg9	2	.0000	.6667	.6167	
O25	1	.3333	.0000	.6517	
O26	1	.3333	.3333	.6517	
O27	1	.3333	.6667	.6517	
O28	1	.6667	.8333	.7500	
O29	1	.4167	.0833	.7500	
O30	1	.9167	.0833	.7500	
Si7	3	.6667	.0000	.7707	
Si8	3	.6667	.6667	.7707	
O31	1	.6667	.3333	.8288	
O32	1	.6667	.0000	.8288	
O33	1	.6667	.6667	.8288	
Mg10	2	.3333	.0000	.8666	
Mg11	2	.3333	.3333	.8666	
Mg12	2	.3333	.6667	.8666	
O34	1	.0000	.0000	.9017	
O35	1	.0000	.3333	.9017	
O36	1	.0000	.6667	.9017	

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TITL 4m90modell3.ins as C1
CELL 0.71073 5.314 9.204 28.428 90.00 90.00 90.00
ZERR 2.00 0.001 0.002 0.004 0.00 0.00 0.00
LATT -7
SFAC O MG SI
UNIT 72 24 16
O1 1 10.2500 .2500 10.0000 Four-layer, alpha = 90
O2 1 10.0000 .5000 10.0000
O3 1 10.7500 .2500 10.0000 Model 13
Si1 3 .0000 .3333 .0207
Si2 3 .0000 .6667 .0207 0,0,-b/3,+b/3
O4 1 .0000 .0000 .0788
O5 1 .0000 .3333 .0788 I,II,I,II
O6 1 .0000 .6667 .0788
Mg1 2 .3333 .0000 .1166 C1
Mg2 2 .3333 .3333 .1166
Mg3 2 .3333 .6667 .1166
O7 1 .6667 .0000 .1517
O8 1 .6667 .3333 .1517
O9 1 .6667 .6667 .1517
O10 1 .5000 .0000 .2500
O11 1 .2500 .2500 .2500
O12 1 .7500 .2500 .2500
Si3 3 .0000 .3333 .2707
Si4 3 .0000 .6667 .2707
O13 1 .0000 .0000 .3288
O14 1 .0000 .3333 .3288
O15 1 .0000 .6667 .3288
Mg4 2 .6667 .0000 .3666
Mg5 2 .6667 .3333 .3666
Mg6 2 .6667 .6667 .3666
O16 1 .3333 .0000 .4017
O17 1 .3333 .3333 .4017
O18 1 .3333 .6667 .4017
O19 1 .2500 .2500 .5000
O20 1 .0000 .5000 .5000
O21 1 .7500 .2500 .5000
Si5 3 .0000 .3333 .5207
Si6 3 .0000 .6667 .5207
O22 1 .0000 .0000 .5789
O23 1 .0000 .3333 .5789
O24 1 .0000 .6667 .5789
Mg7 2 .3333 .0000 .6167
Mg8 2 .3333 .3333 .6167
Mg9 2 .3333 .6667 .6167
O25 1 .6667 .0000 .6517
O26 1 .6667 .3333 .6517
O27 1 .6667 .6667 .6517
O28 1 .0000 .1667 .7500
O29 1 .2500 .4167 .7500
O30 1 .7500 .4167 .7500
Si7 3 .0000 .0000 .7707
Si8 3 .0000 .3333 .7707
O31 1 .0000 .6667 .8288
O32 1 .0000 .0000 .8288
O33 1 .0000 .3333 .8288
Mg10 2 .6667 .0000 .8666
Mg11 2 .6667 .3333 .8666
Mg12 2 .6667 .6667 .8666
O34 1 .3333 .0000 .9017
O35 1 .3333 .3333 .9017
O36 1 .3333 .6667 .9017

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TITL 4m90modell14.ins as C1
CELL 0.71073 5.314 9.204 28.428 90.00 90.00 90.00
ZERR      2.00      0.001  0.002      0.004  0.00  0.00  0.00
LATT  -7
SFAC  O MG SI
UNIT  72 24 16
O1     1    10.2500 .2500 10.0000      Four-layer, alpha = 90
O2     1    10.0000 .5000 10.0000
O3     1    10.7500 .2500 10.0000      Model 14
Si1    3     .0000 .3333 .0207
Si2    3     .0000 .6667 .0207      0, -b/3, -b/3, -b/3
O4     1     .0000 .0000 .0788
O5     1     .0000 .3333 .0788      I, I, II, II
O6     1     .0000 .6667 .0788
Mg1    2     .3333 .0000 .1166      C1
Mg2    2     .3333 .3333 .1166
Mg3    2     .3333 .6667 .1166
O7     1     .6667 .0000 .1517
O8     1     .6667 .3333 .1517
O9     1     .6667 .6667 .1517
O10    1     .5000 .0000 .2500
O11    1     .2500 .2500 .2500
O12    1     .7500 .2500 .2500
Si3    3     .0000 .3333 .2707
Si4    3     .0000 .6667 .2707
O13    1     .0000 .0000 .3288
O14    1     .0000 .3333 .3288
O15    1     .0000 .6667 .3288
Mg4    2     .3333 .0000 .3666
Mg5    2     .3333 .3333 .3666
Mg6    2     .3333 .6667 .3666
O16    1     .6667 .0000 .4017
O17    1     .6667 .3333 .4017
O18    1     .6667 .6667 .4017
O19    1     .0000 .1667 .5000
O20    1     .7500 .9167 .5000
O21    1     .2500 .9167 .5000
Si5    3     .0000 .0000 .5207
Si6    3     .0000 .3333 .5207
O22    1     .0000 .6667 .5789
O23    1     .0000 .0000 .5789
O24    1     .0000 .3333 .5789
Mg7    2     .6667 .0000 .6167
Mg8    2     .6667 .3333 .6167
Mg9    2     .6667 .6667 .6167
O25    1     .3333 .0000 .6517
O26    1     .3333 .3333 .6517
O27    1     .3333 .6667 .6517
O28    1     .0000 .8333 .7500
O29    1     .2500 .0833 .7500
O30    1     .7500 .0833 .7500
Si7    3     .0000 .0000 .7707
Si8    3     .0000 .6667 .7707
O31    1     .0000 .3333 .8288
O32    1     .0000 .0000 .8288
O33    1     .0000 .6667 .8288
Mg10   2     .6667 .0000 .8666
Mg11   2     .6667 .3333 .8666
Mg12   2     .6667 .6667 .8666
O34    1     .3333 .0000 .9017
O35    1     .3333 .3333 .9017
O36    1     .3333 .6667 .9017

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