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Synthesis and characterization of amphiboles along the tremolite–glaucophane join.

Table 6 – Supplementary crystallographic data. Single-crystal refinements (SREF) of samples WIN 9-1 and WIN 4-2

WIN 9-1

a = 9.8076(9) *b* = 18.0004(17) *c* = 5.2804(5) Å beta = 104.575(2)° *V* = 902.21 Å^3

Atom coordinates, refined site-scattering values (ss, epfu), atomic-displacement parameters (B_{eq}, Å^2; β_{ij})

Site	ss	x/*a*	y/*b*	z/*c*	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	32.00	0.11079	0.08660	0.21658	0.88	0.0020	0.0008	0.0080	-0.00012	0.0010	-0.0001
O(2)	32.00	0.11901	0.17091	0.72730	0.97	0.0029	0.0009	0.0079	0.00019	0.0020	0.0002
O(3)	16.00	0.10967	0.00000	0.71368	1.12	0.0027	0.0009	0.0117	0.00000	0.0012	0.0000
O(4)	32.00	0.36549	0.24850	0.79236	1.24	0.0042	0.0009	0.0103	-0.00020	0.0023	-0.0001
O(5)	32.00	0.34739	0.13453	0.09805	1.15	0.0029	0.0011	0.0092	0.00001	0.0012	0.0008
O(6)	32.00	0.34379	0.11802	0.58993	1.05	0.0030	0.0009	0.0086	0.00016	0.0015	-0.0007
O(7)	16.00	0.33697	0.00000	0.28829	1.14	0.0036	0.0004	0.0145	0.00000	0.0011	0.0000
T(1)	55.80	0.28068	0.08468	0.29671	0.71	0.0020	0.0006	0.0064	-0.00002	0.0013	-0.0001
T(2)	56.00	0.28869	0.17169	0.80393	0.82	0.0024	0.0007	0.0070	-0.00016	0.0011	-0.0000
M(1)	24.00	0.00000	0.08826	0.50000	0.78	0.0024	0.0006	0.0066	0.00000	0.0013	0.0000
M(2)	24.06	0.00000	0.17748	0.00000	0.84	0.0024	0.0008	0.0072	0.00000	0.0018	0.0000
M(3)	24.00	0.00000	0.00000	0.00000	0.83	0.0028	0.0005	0.0081	0.00000	0.0014	0.0000
M(4)	34.56	0.00000	0.27719	0.50000	1.08	0.0035	0.0009	0.0101	0.00000	0.0036	0.0000
*A*2	2.38	0.00000	0.47927	0.00000	3.20						
H	2.00	0.20284	0.00000	0.76357	1.89						

R$_{3\sigma}$ = 3.51 (806 refl.) $R_{5\sigma}$ = 2.69 (614 refl.) R_{all} = 7.20 (1369 refl.) *F*(000)= 805.58 limited to θ = 30°

Selected interatomic distances (Å) and angles (°). Values of tetrahedral (T) and octahedral (O) quadratic elongation (QE) and angular variance (AV) are calculated according to Robinson et al. (1971). DELTA is calculated according to Brown and Shannon (1973)

T(1)-O(1)	1.613		*T*(2)-O(2)	1.611		*M*(4)-O(2)	2.400		*M*(1)-O(1)	2.059		*M*(2)-O(1)	2.131		*M*(3)-O(1)	2.072
-O(5)	1.637		-O(4)	1.583		-O(4)	2.316		-O(2)	2.076		-O(2)	2.073		-O(3)	2.064
-O(6)	1.630		-O(5)	1.656		-O(5)	2.770		-O(3)	2.084		-O(4)	1.997		H-O(3)	0.885
-O(7)	1.626		-O(6)	1.676		-O(6)	2.549		<*M*(1)-O>	2.073		<*M*(2)-O>	2.067		<*M*(3)-O>	2.069
<*T*(1)-O>	1.626		<*T*(2)-O>	1.631		<*M*(4)-O>	2.508		VOL.	11.685		VOL.	11.642		VOL.	11.557
VOL.	2.205		VOL.	2.212					OQE	1.0112		OQE	1.0082		OQE	1.0148
TQE	1.0010		TQE	1.0053					OAV	36.83		OAV	25.61		OAV	48.23
TAV	4.13		TAV	21.70					DELTA	0.254		DELTA	6.963		DELTA	0.031

A -O(5)	2.958	*A*(2)-O(5)	2.664	*T*(1)-*T*(2)-*T*(1)	118.58
-O(6)	3.143	-O(6)	2.904	*T*(1)-O(5)-*T*(2)	136.25
-O(7)	2.469	-O(7)	2.498	*T*(1)-O(6)-*T*(2)	137.95
<*A* -O>	2.934	<*A*(2)-O>	2.688	*T*(1)-O(7)-*T*(1)	139.34
				M(1)-*M*(2)	3.090

WIN 4-2

a = 9.7739(11) *b* = 17.9636(20) *c* = 5.2659(6) Å beta = 104.423(3)° *V* = 895.42 Å^3

Atom coordinates, refined site-scattering values (ss, epfu), atomic-displacement parameters (B_{eq}, Å^2; β_{ij})

Site	ss	x/*a*	y/*b*	z/*c*	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	32.00	0.11062	0.08673	0.21645	0.65	0.0021	0.0007	0.0034	-0.0001	0.0008	0.0001
O(2)	32.00	0.11904	0.17120	0.72635	0.72	0.0019	0.0006	0.0063	0.0002	0.0009	0.0001
O(3)	16.00	0.10974	0.00000	0.71485	0.76	0.0021	0.0007	0.0059	0.0000	0.0014	0.0000
O(4)	32.00	0.36571	0.24868	0.79115	0.94	0.0037	0.0005	0.0088	-0.0004	0.0023	-0.0001
O(5)	32.00	0.34784	0.13441	0.09800	0.94	0.0032	0.0009	0.0057	0.0001	0.0015	0.0010
O(6)	32.00	0.34347	0.11794	0.58877	0.86	0.0027	0.0010	0.0034	0.0001	0.0009	-0.0010
O(7)	16.00	0.33775	0.00000	0.28706	0.96	0.0029	0.0005	0.0129	0.0000	0.0024	0.0000
T(1)	56.00	0.28063	0.08459	0.29511	0.46	0.0018	0.0004	0.0029	0.0000	0.0009	-0.0001
T(2)	55.80	0.28941	0.17146	0.80351	0.49	0.0020	0.0004	0.0025	-0.0001	0.0008	0.0001
M(1)	24.00	0.00000	0.08830	0.50000	0.57	0.0026	0.0004	0.0024	0.0000	0.0012	0.0000
M(2)	24.33	0.00000	0.17747	0.00000	0.65	0.0022	0.0005	0.0053	0.0000	0.0011	0.0000
M(3)	12.31	0.00000	0.00000	0.00000	0.63	0.0027	0.0003	0.0046	0.0000	0.0009	0.0000
M(4)	34.26	0.00000	0.27693	0.50000	0.95	0.0037	0.0008	0.0078	0.0000	0.0040	0.0000
A	2.90	0.00000	0.50000	0.00000	6.17						
H	2.00	0.19245	0.00000	0.74231	1.31						

$R_{3\sigma}$ = 4.38 (1020 refl.) $R_{5\sigma}$ = 3.82 (863 refl.) R_{all} = 6.34 (1837 refl.) $F(000)$= 805.58 limited to θ = 35°

Selected interatomic distances (Å) and angles (°). Values of tetrahedral (T) and octahedral (O) quadratic elongation (QE) and angular variance (AV) are calculated according to Robinson et al. (1971). DELTA is calculated according to Brown and Shannon (1973)

T(1)-O(1)	1.610	*T*(2)- (O2)	1.613	*M*(4)- (O2)	2.386	*M*(1)-O(1)	2.050	*M*(2)-O(1)	2.124	*M*(3)-O(1)	2.069
-O(5)	1.628	-O(4)	1.584	-O(4)	2.299	-O(2)	2.074	-O(2)	2.068	-O(3)	2.051
-O(6)	1.629	-O(5)	1.653	-O(5)	2.768	-O(3)	2.084	-O(4)	1.993	H-O(3)	0.785
-O(7)	1.623	-O(6)	1.667	-O(6)	2.546	<*M*(1)-O>	2.069	<*M*(2)-O>	2.062	<*M*(3)-O>	2.063
<*T*(1)-O>	1.622	<*T*(2)-O>	1.629	<*M*(4)-O>	2.500	VOL.	11.618	VOL.	11.559	VOL.	11.452
VOL.	2.188	VOL.	2.205			OQE	1.0113	OQE	1.0081	OQE	1.0150
TQE	1.0011	TQE	1.0047			OAV	37.17	OAV	25.22	OAV	48.71
TAV	4.69	TAV	18.79			DELTA	0.462	DELTA	6.748	DELTA	0.169

A -O(5)	2.948	*A*(2)-O(5)	3.005	*T*(1)-*T*(2)-*T*(1)	118.62
-O(6)	3.141	-O(6)	3.619	*T*(1)-O(5)-*T*(2)	136.02
-O(7)	2.448	-O(7)	5.476	*T*(1)-O(6)-*T*(2)	138.38
<*A* -O>	2.925	<*A*(2-O>	4.034	*T*(1)-O(7)-*T*(1)	138.86
				M(1)-*M*(2)	3.082