

Supplementary

**Tetrahedral aluminum in tourmaline from
a spinel-pargasite-metamorphosed mafic-ultramafic rock**

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Table S1. Site-scattering values (epfu) and assigned site occupancies
in the studied tourmaline (sample 1AD-23).

Site	Site population (apfu) from EMPA	Site scattering (epfu)		
		Refined	Calculated	Difference, %
<i>X</i>	Ca _{0.95} Na _{0.03} □ _{0.02}	19.33	19.93	12.0
<i>Y</i>	Mg _{1.08} Al _{0.98} Fe ²⁺ _{0.50} Fe ³⁺ _{0.43}	16.63	16.94	5.3
<i>Z</i>	Al _{5.91} Fe ³⁺ _{0.09}	12.81	13.16	4.6

Table S2. Site-scattering values (epfu) and assigned site occupancies
in the studied tourmaline (sample 2AD-23).

Site	Site population (apfu) from EMPA	Site scattering (epfu)		
		Refined	Calculated	Difference, %
<i>X</i>	Ca _{0.89} Na _{0.11}	19.01	18.72	5.3
<i>Y</i>	Mg _{1.55} Al _{0.80} Fe ²⁺ _{0.34} Fe ³⁺ _{0.31}	15.30	15.75	7.1
<i>Z</i>	Al _{5.51} Mg _{0.44} Fe ³⁺ _{0.05}	13.04	13.19	2.0

Table S3. Bond valence values for the studied tourmaline (sample 1AD-23).

	<i>X</i>	<i>Y</i>	<i>Z</i>	<i>T</i>	<i>B</i>	Σ
O1(<i>W</i>)		³ ×→ 0.507				1.521
O2	0.205 ↓×3	² ×→ 0.398 ↓×2			0.947	1.948
O3(<i>V</i>)		0.266	² ×→ 0.396			1.058
O4	0.158 ↓×3			² ×→ 0.911		1.980
O5	0.127 ↓×3			² ×→ 0.959		2.045
O6		0.483 ↓×2	0.556	0.978		2.017
O7			0.547 0.478	1.002		2.027
O8			0.509 0.477		0.995 ↓×2	1.981
BVS	1.470	2.535	2.963	3.850	2.937	

Table S4. Bond valence values for the studied tourmaline (sample 2AD-23).

	<i>X</i>	<i>Y</i>	<i>Z</i>	<i>T</i>	<i>B</i>	Σ
O1(<i>W</i>)		$3 \times \rightarrow 0.513$				1.539
O2	$0.212 \downarrow \times 3$	$2 \times \rightarrow 0.397 \downarrow \times 2$			0.958	1.964
O3(<i>V</i>)		0.273	$2 \times \rightarrow 0.399$			1.071
O4	$0.155 \downarrow \times 3$			$2 \times \rightarrow 0.910$		1.975
O5	$0.122 \downarrow \times 3$			$2 \times \rightarrow 0.960$		2.042
O6		$0.476 \downarrow \times 2$	0.548	0.992		2.016
O7			0.538 0.468	1.017		2.022
O8			0.512 0.482		$0.992 \downarrow \times 2$	1.986
BVS	1.468	2.532	2.947	3.879	2.942	