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A transitional structural state and anomalous Fe-Mg order-disorder in Mg-rich
orthopyroxene, $(\text{Mg}_{0.75}\text{Fe}_{0.25})_2\text{Si}_2\text{O}_6$

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For deposit: Table 7

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Table 7. Amplitudes (\AA) and orientations of major axes of thermal ellipsoids in the En₇₅Fs₂₅ orthopyroxene at various temperatures

Atom	Eillipsoid	296K	1000K	1100K	1200K	1300K
	axis (r_i)					
M1	RMS*	0.074	0.121	0.130	0.142	0.147
	a**	70.8	69.4	62.2	69.2	65.7
r ₁	b	92.1	91.4	94.1	94.3	99.3
	c	19.4	20.6	28.1	21.3	26.2
	RMS	0.075	0.138	0.149	0.165	0.174
	a	101.2	88.5	98.0	92.0	97.3
r ₂	b	168.6	177.4	172.0	175.6	170.
	c	88.6	92.1	90.4	93.9	96.8
	RMS	0.087	0.151	0.165	0.173	0.178
	a	157.5	159.3	150.9	159.1	154.5
r ₃	b	78.8	92.1	83.2	89.5	86.2
	c	70.7	67.5	61.9	69.1	64.8

Table 7. (continued)

M2	RMS	0.075	0.133	0.146	0.158	0.166
r_1	a	57.9	59.6	62.5	58.0	59.6
	b	81.6	87.6	90.3	86.6	83.4
	c	33.5	30.5	27.5	32.2	31.2
r_2	RMS	0.086	0.160	0.171	0.186	0.206
	a	80.2	75.5	74.5	75.2	74.9
	b	18.8	18.5	17.4	19.9	22.4
r_3	c	105.9	101.2	97.7	103.0	106.1
	RMS	0.105	0.196	0.206	0.224	0.228
	a	146.0	145.6	147.7	144.0	145.3
SiA	b	73.3	71.7	72.6	70.4	68.7
	c	61.4	62.0	63.8	61.1	64.0
	RMS	0.072	0.114	0.116	0.127	0.134
r_1	a	40.0	62.0	48.6	65.3	33.6
	b	50.4	51.1	57.9	62.6	61.0
	c	85.3	51.7	58.0	38.4	74.6
r_2	RMS	0.074	0.117	0.120	0.129	0.137
	a	92.4	52.5	65.8	42.1	73.2
	b	79.8	73.8	70.3	71.0	88.7
r_3	c	169.5	138.0	148.0	125.9	163.1
	RMS	0.081	0.132	0.139	0.148	0.159
	a	129.9	50.2	51.0	58.4	62.0
	b	41.5	136.6	141.0	145.7	150.9
	c	80.6	75.4	90.3	78.2	83.0

Table 7. (continued)

SiB	RMS	0.071	0.107	0.115	0.129	0.136
r_1	a	55.1	46.4	44.9	40.6	55.1
	b	116.3	111.9	93.1	100.4	110.2
	c	46.4	51.6	45.2	51.3	41.9
r_2	RMS	0.074	0.121	0.133	0.141	0.150
	a	108.7	62.7	72.9	78.9	65.0
	b	153.5	116.1	21.7	148.8	25.6
r_3	c	108.1	140.1	103.0	118.7	84.6
	RMS	0.081	0.131	0.133	0.146	0.159
	a	139.0	124.2	130.0	128.4	65.0
O1A	b	87.5	144.8	68.7	119.1	25.6
	c	49.1	82.4	47.6	52.1	84.6
	RMS	0.066	0.116	0.131	0.124	0.148
r_1	a	151.0	156.4	173.8	167.3	165.2
	b	109.2	105.1	95.3	92.5	82.8
	c	69.1	72.2	86.7	77.6	77.1
r_2	RMS	0.085	0.138	0.148	0.153	0.167
	a	82.1	108.5	89.9	102.3	97.5
	b	150.9	89.9	123.2	91.1	59.3
r_3	c	117.8	161.5	146.8	167.6	148.2
	RMS	0.098	0.160	0.160	0.179	0.185
	a	62.3	104.2	83.8	87.3	77.3
	b	111.0	15.1	146.3	177.3	31.7
	c	36.0	85.2	57.0	89.5	61.5

Table 7. (continued)

O1B	RMS	0.078	0.113	0.123	0.138	0.142
r_1	a	17.3	22.9	19.7	30.1	18.7
	b	101.8	79.1	85.8	66.5	87.8
	c	77.5	70.1	70.8	72.3	72.0
r_2	RMS	0.085	0.145	0.153	0.165	0.179
	a	75.2	78.5	74.1	74.8	79.8
	b	20.6	58.9	66.2	80.9	49.1
r_3	c	104.0	146.4	150.8	162.2	137.3
	RMS	0.092	0.165	0.174	0.176	0.204
	a	98.7	109.5	101.3	115.3	105.6
r_4	b	73.3	33.4	24.2	25.4	41.4
	c	19.0	64.0	68.9	88.1	52.9
	RMS	0.082	0.130	0.131	0.135	0.139
r_5	a	59.7	59.4	122.6	55.3	57.2
	b	30.3	31.1	147.3	35.0	33.3
	c	90.4	85.1	88.5	85.9	84.7
r_6	RMS	0.091	0.152	0.161	0.169	0.190
	a	117.6	105.4	104.2	103.2	99.5
	b	74.7	75.6	82.7	76.1	77.7
r_7	c	147.7	158.7	163.9	160.6	164.4
	RMS	0.111	0.178	0.202	0.218	0.229
	a	136.7	145.0	143.7	142.2	145.5
r_8	b	64.5	63.1	58.4	58.6	59.6
	c	57.7	69.3	74.0	71.1	75.4

Table 7. (continued)

O2B	RMS	0.076	0.110	0.116	0.132	0.154
r_1	a	60.2	61.0	60.0	56.3	125.6
	b	146.7	139.9	146.1	139.6	35.7
	c	76.1	64.9	75.7	70.5	88.0
r_2	RMS	0.094	0.146	0.168	0.182	0.180
	a	108.9	84.1	75.1	71.3	89.3
	b	115.8	115.6	97.5	100.0	87.0
r_3	c	147.1	153.6	163.2	158.6	177.0
	RMS	0.107	0.188	0.190	0.211	0.231
	a	143.6	150.3	34.2	39.9	35.6
O3A	b	109.9	118.5	57.2	51.4	54.5
	c	60.9	82.5	81.5	81.5	87.7
	RMS	0.076	0.113	0.119	0.118	0.129
r_1	a	89.9	83.8	86.8	86.9	83.9
	b	64.5	65.5	65.2	67.7	63.7
	c	25.5	25.4	25.1	22.6	27.1
r_2	RMS	0.097	0.138	0.165	0.172	0.187
	a	169.1	10.7	6.3	169.9	6.9
	b	80.2	100.6	86.4	79.9	90.0
r_3	c	94.6	91.9	95.2	90.8	96.9
	RMS	0.114	0.193	0.209	0.234	0.258
	a	100.8	98.8	84.6	99.6	86.9
	b	152.4	153.0	154.9	155.3	153.7
	c	65.0	64.7	65.5	67.4	63.9

Table 7. (continued)

O3B	RMS	0.072	0.120	0.131	0.144	0.143
r_1	a	69.8	95.0	92.3	43.2	90.6
	b	63.5	57.6	55.2	61.4	55.6
	c	34.4	32.9	34.9	60.6	34.3
r_2	RMS	0.089	0.152	0.161	0.154	0.179
	a	70.9	24.4	14.5	48.1	8.7
	b	39.9	67.4	77.0	109.7	82.5
r_3	c	123.5	98.6	96.3	131.7	94.4
	RMS	0.103	0.190	0.205	0.249	0.315
	a	151.6	66.2	75.6	81.3	81.3
r_3	b	62.6	138.7	142.2	144.2	144.6
	c	83.2	58.6	55.9	55.6	55.9

* RMS--root mean square amplitude (\AA).

** a,b,c---angles ($^\circ$) of r_i with unit cell edges a , b and c , respectively.