Crystal structure of the disordered non-centrosymmetric compound $Fe_{0.43}Mo_{2.56}SbO_{9.5}$

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Table S1. Qualitative EDS analyses on single crystals were performed in a scanning electron microscope (JEOL-7000F) showing that all the intended elements are present in $Fe_{0.43}Mo_{2.56}SbO_{9.5}$. Average composition is calculated considering several points in a crystal.

EDS data (at %)			Average (at %)			Expected values (at %)		
Fe	Mo	Sb	Fe	Mo	Sb	Fe	Mo	Sb
13.9	54.4	31.7	10.6	61.3	28.1	10.8	64.0	25.0
8.6	61.4	30						
10.4	60.8	28.8						
12.5	58.4	29.1						
7.6	66.2	26.2						
7.2	69.8	23						
9.7	54.8	35.5						
15.1	64.3	20.6						

Table S2 (a) Structural parameters of the cations and **(b)** anions in $Fe_{0.43}Mo_{2.56}SbO_{9.5}$ (Occ. = Occupation factor).

(a)

Atom	x	y	z	U^{equiv} (Å^2)	Occ
Sb1	− 0.0057 (5)	0.1957 (1)	0.4887 (1)	0.0269 (2)	1
Mo1	0.0733 (3)	− 0.4944 (3)	0.7699 (2)	0.0066 (2)	0.72
Fe1	0.0733 (3)	− 0.4944 (3)	0.7699 (2)	0.0066 (2)	0.12
Mo1a	− 0.1042 (8)	− 0.4946 (13)	0.7723 (4)	0.0001	0.13
Fe1a	− 0.1042 (8)	− 0.4946 (13)	0.7723 (4)	0.0001	0.02
Mo2	− 0.0970 (3)	− 0.0094 (2)	0.2607 (2)	0.0056 (2)	0.64
Fe2	− 0.0970 (3)	− 0.0094 (2)	0.2607 (2)	0.0056 (2)	0.11
Mo2a	− 0.0557 (6)	− 0.0131 (7)	0.2586 (3)	0.0039 (4)	0.21
Fe2a	− 0.0557 (6)	− 0.0131 (7)	0.2586 (3)	0.0039 (4)	0.04
Mo3	− 0.0989 (3)	0.2639 (1)	0.0193 (2)	0.0108 (2)	0.86
Fe3	− 0.0989 (3)	0.2639 (1)	0.0193 (2)	0.0108 (2)	0.14

(b)

Atom	x	y	z	U^{equiv} (Å^2)	Occ
O1	0.4925 (15)	0.4948 (11)	0.2610 (6)	0.0193 (12)	1
O2	− 0.5261 (14)	− 0.0063 (14)	0.22527 (6)	0.0135 (9)	1
O3	− 0.5319 (13)	0.2555 (5)	0.0081 (7)	0.0116 (14)	1
O4	− 0.0294 (21)	0.4213 (9)	0.1298 (6)	0.0140 (11)	1
O5	0.0125 (16)	0.0523 (9)	0.1170 (6)	0.0122 (11)	1
O6	− 0.0063 (33)	0.7462 (6)	0.2347 (9)	0.0178 (21)	1
O7	− 0.0077 (27)	0.2391 (7)	0.3216 (9)	0.0150 (17)	1
O8	0.0041 (23)	0.5622 (12)	0.4161 (7)	0.0170 (13)	1
O9	− 0.0404 (16)	− 0.0556 (9)	0.4165 (6)	0.0076 (10)	1
O10	− 0.4765 (57)	0.2321 (16)	0.4820 (17)	0.0267 (35)	0.5