Supporting Material for the paper “On the structure and properties of the $\text{Mo}_3\text{Nb}_2\text{O}_{14}$ oxide”.

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Table 1 Full chemical analysis data for the specimens prepared

Sample	Mo, wt %	Nb, wt %	Nb/Mo at.	Oxygen, calculated.	100% - sum of the elements
NbMo1	9.94	60.13	6.25	29.6238	0.31
NbMo2	8.80	61.42	6.98	29.5865	0.19
NbMo3	11.21	58.37	5.38	29.5377	0.89
NbMo4					
NbMo5					
NbMo6					
NbMo7	39.71	28.33	0.74	31.4453	0.47
NbMo8	40.56	27.72	0.71	31.6576	0.06
NbMo9	38.59	29.66	0.79	31.4652	0.29
NbMo10	40.90	27.26	0.67	31.6410	0.20

Tale 2 Final atomic fractional coordinates, s.o.f. and Biso obtained by Rietveld refinement for the NbMo10 specimen

Atom	Wyck.	s.o.f.	x	y	z	B/ Å ²	
Mo1	8k	0.500000	0.300500	0.199500	0.425000	0.72(3)	
Mo2	8k	0.500000	0.403300	0.096700	0.425000	0.69(3)	
Mo3	16l	0.500000	0.050000	0.338800	0.425000	0.75(3)	
Mo4	16l	0.500000	0.082100	0.077000	0.425000	0.65(3)	
Mo5	16l	0.500000	0.159000	0.219000	0.425000	0.79(3)	
Mo6	16l	0.500000	0.240800	0.071300	0.425000	0.70(3)	
O1	4g	1.000000	0.297000	0.203000	0.000000	0.25(3)	
O2	4g	1.000000	0.399000	0.101000	0.000000	0.25(3)	
O3	8i	1.000000	0.048000	0.347000	0.000000	0.25(3)	
O4	8i	1.000000	0.095000	0.077000	0.000000	0.25(3)	
O5	8i	1.000000	0.156000	0.220000	0.000000	0.25(3)	
O6	8i	1.000000	0.248000	0.079000	0.000000	0.25(3)	
O7	4h	1.000000	0.097000	0.403000	0.500000	0.25(3)	
O8	4h	1.000000	0.233000	0.267000	0.500000	0.25(3)	
O9	8j	1.000000	0.271000	0.002000	0.500000	0.25(3)	
O10	8j	1.000000	0.033000	0.084000	0.500000	0.25(3)	
O11	8j	1.000000	0.105000	0.161000	0.500000	0.25(3)	
O12	8j	1.000000	0.111000	0.287000	0.500000	0.25(3)	
O13	8j	1.000000	0.169000	0.058000	0.500000	0.25(3)	
O14	8j	1.000000	0.220000	0.160000	0.500000	0.25(3)	
O15	8j	1.000000	0.317000	0.113000	0.500000	0.25(3)	
O16	8j	1.000000	0.389000	0.023000	0.500000	0.25(3)	

Table 3 Cell refinement fit parameters for the solid NbMo10

Lattice parameters:

a/ Å:	23,150(6)
b/ Å:	23,150(6)
c/ Å:	3,998(4)
α °:	90
β °:	90
γ °:	90

Space group :	P 4/m b m (127)
V/ 10 ⁶ pm ³	2142, 07
Density g/cm ³	4,3610

Table 4 General Rietveld Fit Parameters for the specimen NbMo10

Number of variables:	33
Number of constraints:	20
Zero shift/ °2Theta:	0,082(1)
Profile function:	Pseudo Voigt
Background:	Polynomial
R (profile)/ %:	6.85
R (weighted profile)/ %:	7.33

Figure 1. Instrumental linewidth for the BRUKER XRD device used.

Fig. 2. Fragment of the XRD pattern of NbMo10 specimen in the low angles region (strong lines). Red line - experimental curve; blue line – Rietveld fit.

Fig. 3. Fragment of the XRD pattern of NbMo10 specimen in the middle angles region (weak lines). Red line - experimental curve; blue line – Rietveld fit.

Table 5 Selected bond lengths (Å) and angles (°) in the refined Mo₃Nb₂O₁₄ structure^a.

Mo1	- O1	1.703	1 ^b	Mo2	- O2	1.705	1
	- O15	2.061	2		- O16	1.764	2
	- O14	2.098	2		- O15	2.055	2
	- O8	2.230	1		- O2	2.304	1
	- O1	2.302	1		- Mo1	3.366	1
	- Mo6	3.274	2		- Mo2	3.399	1
	- Mo5	3.307	2		- Mo1	3.419	1
	- Mo6	3.329	2	Mo3	- O3	1.711	1
	- Mo5	3.361	2		- O7	1.866	1
	- Mo2	3.366	1		- O12	1.877	1
	- Mo1	3.399	1		- O9	2.001	1
	- Mo2	3.419	1		- O16	2.073	1
					- O3	2.308	1
					- Mo3	3.399	1
Mo4	- O10	1.187	1	Mo6	- O13	1.717	1

Fig. 4 XRD pattern of the NbMo01 specimen (Nb₆MoO₁₈ solid).

Fig. 5. Optical gap for the solids presented in Table 2 as a function of ratio of mean electronegativity (E_{mean}) to the shortest metal –metal distance $d(\text{M-M})$. Nb-Mo oxide is marked by red color.