Synthesis, Structure and Thermal Contraction of a New Low Temperature Polymorph of ZrMo₂O₈
Supplementary Data

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Fractional atomic coordinates of LT-ZrMo₂O₈. Numbers in parentheses are the estimated standard deviation of the last digit derived from Rietveld refinement, and represent an overestimate of the true precision of the determination. Space group Pmn2₁; a=5.87961(1), b=7.31560(5), c=9.13945(5) Å. Temperature factors of structurally related sites (O12/O13/O22/O23) equated.

Site	x/a	y/b	z/c	Biso (Å ²)
Zr1	0.5	0.27673(27)	0.5	0.526(45)
Mo1	0.5	0.94675(22)	0.19028(25)	1.446(39)
O11	0.5	0.78571(41)	0.29206(30)	4.035(69)
O12	0.5	0.15080(27)	0.28422(40)	1.894(45)
O13	0.77334(22)	0.91796(28)	0.07265(25)	1.894(45)
Mo2	0.5	0.42562(24)	0.89323(24)	1.446(39)
O21	0.5	0.22491(50)	-0.01038(40)	3.676(65)
O22	0.5	0.37779(36)	0.71617(31)	1.894(45)
O23	0.74173(26)	0.55794(23)	0.95476(24)	1.894(45)

Bond distances and bond valence sums for LT-ZrMo₂O₈.

	O11	O12	O13*2	O21	O22	O23*2	Valence
Zr1		2.136	2.025		2.054	2.071	4.13
Mo1	1.643	1.775	1.807				6.22
Mo2				1.713	1.753	1.781	6.01
Valence	2.042254	2.013402	2.024864	1.814299	2.242562	2.10163	

Bond Distance and Angles

Bond distances with esds; intrapolyhedral bond angles for ZrO₆ octahedra and MoO₄ tetrahedra; Mo-O-Zr bond angles.

Zr1:0	O22:1	2.0545(28)							
	O13:0	2.0618(22)	88.242(52)						
	O13:0	2.0618(22)	88.03(12)	88.242(52)					
	O23:0	2.0708(16)	175.184(84)	88.706(67)	88.119(49)				
	O23:0	2.0708(16)	94.325(93)	88.706(67)	175.184(84)	88.119(49)			
	O12:1	2.1358(36)	90.861(59)	90.861(59)	92.837(95)	92.837(95)	178.499(72)		
Mo1:0	O11:0	1.6425(35)							
	O12:1	1.7753(32)	108.52(16)						
	O13:0	1.8071(21)	112.911(72)	104.311(80)					
	O13:0	1.8071(21)	113.02(17)	112.911(72)	104.311(80)				
	O21:0	2.6748(41)	74.897(97)	74.897(97)	73.05(13)	178.44(13)			
Mo2:0	O21:0	1.7136(41)							
	O22:1	1.7527(28)	109.39(15)						
	O23:0	1.7812(17)	111.283(45)	109.480(88)					
	O23:0	1.7812(17)	105.86(11)	111.283(45)	109.480(88)				
O12:0	Mo1:1	1.7753(18)							
	Zr1:0	2.13577(79)	145.305(85)						
O13:0	Mo1:1	1.8071(17)							
	Zr1:0	2.0618(16)	145.908(69)						
O22:0	Mo2:1	1.7527(35)							
	Zr1:0	2.0545(29)	167.39(17)						
O23:0	Mo2:1	1.7812(20)							
	Zr1:0	2.0708(20)	173.66(13)						