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SUPPLEMENTARY INFORMATION
High-pressure structures of α- and δ-$ZrMo_2O_8$

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1.

Table 1
Indexed powder pattern of δ-$ZrMo_2O_8$ at 1.64 GPa. Indexing was based on a monoclinic unit cell: a = 9.8054(11), b = 5.9881(6), c = 5.2862(7) Å, β = 93.080(10) °.

h	k	l	$d_{calc.}$	$d_{obs.}$	I/I_0
1	1	0	5.1086	5.1072	22
0	1	1	3.9598	3.9577	23
-1	1	1	3.7234	3.7242	100
2	0	1	3.4970	3.4975	48
0	2	0	2.9941	2.9942	43
3	1	0	2.8657	2.8654	55
0	0	2	2.6393	2.6408	25
0	2	1	2.6043	2.6054	24
4	0	0	2.4478	2.4471	26
-2	0	2	2.3771	2.3773	27
1	1	2	2.3185	2.3202	36
2	0	2	2.2728	2.2713	35
-2	2	2	1.8617	1.8618	35
-1	3	1	1.8404	1.8404	38
-4	2	1	1.8077	1.8073	39
-5	1	1	1.7841	1.7832	26
0	0	3	1.7595	1.7583	28
4	0	2	1.7485	1.7486	30
5	1	1	1.7279	1.7274	32
3	3	0	1.7028	1.7026	33
6	0	0	1.6319	1.6311	27
1	3	2	1.5634	1.5622	30
-5	1	2	1.5590	1.5596	30
-3	1	3	1.5320	1.5319	27
0	2	3	1.5170	1.5170	30
0	4	0	1.4970	1.4970	29
3	1	3	1.4689	1.4691	27
6	2	0	1.4329	1.4324	29
2	4	1	1.3762	1.3762	28
-7	1	1	1.3359	1.3366	29
4	3	2	1.3153	1.3161	25
-1	1	4	1.2865	1.2865	25
-2	4	2	1.2668	1.2668	26
-5	3	2	1.2554	1.2552	26
-4	4	1	1.2493	1.2493	26
-3	3	3	1.2412	1.2413	26
-6	0	3	1.2299	1.2295	25
3	3	3	1.2069	1.2071	26
7	1	2	1.1854	1.1856	26
-1	5	1	1.1614	1.1612	27
-6	2	3	1.1377	1.1380	27
-7	3	1	1.1298	1.1300	26
3	5	0	1.1243	1.1246	25
6	4	0	1.1032	1.1032	24
6	2	3	1.0863	1.0861	21
1	5	2	1.0813	1.0811	21

IUCr macros version 2.0β1: 1999/12/07

Table 2
Unit-cell dimension for α-$ZrMo_2O_8$ and δ-$ZrMo_2O_8$. Standard uncertainties (s.u.'s) are given in parenthesis.

P (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
0.20(3)	10.13792(6)	-	11.71279(15)	-	1042.536(9)
0.32(3)	10.14778(8)	-	11.67799(19)	-	1041.46(2)
0.42(3)	10.13900(8)	-	11.60748(18)	-	1033.382(15)
0.56(3)	10.14228(11)	-	11.5334(3)	-	1027.46(3)
0.63(3)	10.13168(10)	-	11.4790(3)	-	1020.46(3)
0.72(3)	10.13748(11)	-	11.4394(3)	-	1018.11(3)
0.80(3)	10.13180(10)	-	11.3876(2)	-	1012.37(3)
0.90(3)	10.12640(10)	-	11.3252(2)	-	1005.75(2)
1.06(3)	10.13080(10)	-	11.2618(2)	-	1000.98(3)
1.18(3)	9.8821(3)	5.96990(20)	5.3888(2)	92.818(3)	317.528(20)
1.48(4)	9.8357(3)	5.98562(17)	5.32343(19)	93.00482)	312.975(17)
1.53(4)	9.8255(3)	5.98981(17)	5.31146(19)	93.039(2)	312.156(18)
1.64(4)	9.7965(3)	5.98424(16)	5.28551(18)	93.068(2)	309.418(17)
1.79(4)	9.7833(3)	5.99226(17)	5.26581(18)	93.116(2)	308.247(18)
1.87(4)	9.7642(3)	5.99021(18)	5.24843(19)	93.140(2)	306.519(19)

Table 3
Refined fractional coordinates of α-$ZrMo_2O_8$ at 0.20 – 0.90 GPa. Standard uncertainties (s.u.'s) are given in parenthesis.

P (GPa)	Atom	x	y	z	U_{iso}
0.20	Zr1	0	0	0	0.0066(15)
	Zr2	1/3	2/3	0.9794(3)	0.0066(15)
	Mo	0.3302(11)	0.3387(11)	0.14702(12)	0.0157(8)
	O1	0.158(4)	0.146(4)	0.105(3)	0.005(2)
	O2	0.322(4)	0.498(3)	0.0910(18)	0.005(2)
	O3	0.529(3)	0.359(3)	0.1215(18)	0.005(2)
	O4	0.318(5)	0.340(6)	0.2889(5)	0.005(2)
0.32	Zr1	0	0	0	0.0021(14)
	Zr2	1/3	2/3	0.9752(4)	0.0021(14)
	Mo	0.3298(13)	0.3375(13)	0.14777(14)	0.0137(8)
	O1	0.160(5)	0.150(5)	0.097(2)	0.005(2)
	O2	0.334(6)	0.507(4)	0.0923(18)	0.005(2)
	O3	0.523(3)	0.352(3)	0.1298(11)	0.005(2)
	O4	0.317(5)	0.345(5)	0.2909(6)	0.005(2)
0.42	Zr1	0	0	0	0.0026(14)
	Zr2	1/3	2/3	0.9744(4)	0.0026(14)
	Mo	0.3296(13)	0.3364(13)	0.15044(16)	0.0126(8)
	O1	0.166(7)	0.159(6)	0.0799(18)	0.003(2)
	O2	0.342(9)	0.516(5)	0.0893(17)	0.003(2)
	O3	0.530(3)	0.343(4)	0.1330(12)	0.003(2)
	O4	0.319(4)	0.347(5)	0.2842(8)	0.003(2)
0.56	Zr1	0	0	0	0.0057(16)
	Zr2	1/3	2/3	0.9740(5)	0.0057(16)
	Mo	0.3295(15)	0.3367(24)	0.1512(2)	0.0117(11)
	O1	0.167(7)	0.163(7)	0.078(2)	0.002(3)
	O2	0.341(10)	0.517(6)	0.0909(19)	0.002(3)
	O3	0.531(3)	0.341(6)	0.1338(16)	0.002(3)
	O4	0.317(5)	0.345(5)	0.2846(10)	0.002(3)
0.63	Zr1	0	0	0	0.0023(14)
	Zr2	1/3	2/3	0.9737(5)	0.0023(14)
	Mo	0.3298(15)	0.3369(15)	0.1515(2)	0.0132(10)
	O1	0.165(7)	0.162(6)	0.081(2)	0.003(3)
	O2	0.343(8)	0.517(4)	0.0934(19)	0.003(3)
	O3	0.530(3)	0.339(6)	0.1353(13)	0.003(3)
	O4	0.316(5)	0.345(5)	0.2870(9)	0.003(3)
0.72	Zr1	0	0	0	0.0025(14)
	Zr2	1/3	2/3	0.9727(5)	0.0025814)
	Mo	0.3296(15)	0.3370(15)	0.1520(2)	0.0130(9)
	O1	0.166(7)	0.161(7)	0.080(2)	0.010(3)
	O2	0.338(11)	0.515(6)	0.095(2)	0.010(3)
	O3	0.530(3)	0.340(6)	0.1329(14)	0.010(3)
	O4	0.315(5)	0.344(6)	0.2876(9)	0.010(3)
0.80	Zr1	0	0	0	0.0027(14)
	Zr2	1/3	2/3	0.9718(4)	0.0027(14)
	Mo	0.3290(12)	0.3371(11)	0.1525(2)	0.0147(8)
	O1	0.170(6)	0.162(6)	0.0797(17)	0.009(2)
	O2	0.342(8)	0.515(4)	0.0979(18)	0.009(2)
	O3	0.531(3)	0.339(5)	0.1362(13)	0.009(2)
	O4	0.313(4)	0.341(5)	0.2868(8)	0.009(2)
0.90	Zr1	0	0	0	0.0039(17)
	Zr2	1/3	2/3	0.9717(4)	0.0039(17)
	Mo	0.3283(11)	0.3380(10)	0.1542(3)	0.0148(9)
	O1	0.170(5)	0.164(5)	0.0832(18)	0.001(2)
	O2	0.343(6)	0.519(3)	0.1045(17)	0.001(2)
	O3	0.527(3)	0.336(5)	0.1409(12)	0.001(2)
	O4	0.315(4)	0.337(5)	0.2884(8)	0.001(2)

Table 4
Refined fractional coordinates of δ-$ZrMo_2O_8$ at 1.18 – 1.87 GPa. Standard uncertainties (s.u.'s) are given in parenthesis.

P (GPa)	Atom	x	y	z	U_{iso}
1.18	Zr	0	0	0	0.025(3)
	Mo	0.3297(5)	0	0.3088(8)	0.0063(17)
	O1	0.1130(13)	-0.256(3)	0.857(3)	0.005(3)
	O2	0.1279(15)	0	0.238(3)	0.005(3)
	O3	0.3798(14)	0	0.582(3)	0.005(3)
1.48	Zr	0	0	0	0.023(3)
	Mo	0.3305(5)	0	0.3109(7)	0.0070(16)
	O1	0.1117(11)	-0.247(2)	0.853(2)	0.009(3)
	O2	0.1312(13)	0	0.254(2)	0.009(3)
	O3	0.3740(12)	0	0.602(3)	0.009(3)
1.53	Zr	0	0	0	0.021(3)
	Mo	0.3309(5)	0	0.3144(7)	0.0033817)
	O1	0.1105(12)	-0.248(3)	0.851(2)	0.009(3)
	O2	0.1301(13)	0	0.2562(2)	0.009(3)
	O3	0.3755(12)	0	0.612(3)	0.009(3)
1.64	Zr	0	0	0	0.017(3)
	Mo	0.3302(5)	0	0.3118(7)	0.0098(16)
	O1	0.1111(10)	-0.246(2)	0.848(2)	0.002(3)
	O2	0.1334(13)	0	0.2574(20)	0.002(3)
	O3	0.3738(11)	0	0.609(2)	0.002(3)
1.79	Zr	0	0	0	0.010(3)
	Mo	0.3307(5)	0	0.3131(8)	0.0140(17)
	O1	0.1136(10)	-0.244(2)	0.848(2)	0.001(3)
	O2	0.1334(13)	0	0.2572(20)	0.001(3)
	O3	0.3717(11)	0	0.618(2)	0.001(3)
1.87	Zr	0	0	0	0.010(3)
	Mo	0.3310(5)	0	0.3149(9)	0.0153(18)
	O1	0.1134(11)	-0.2247(2)	0.856(3)	0.005(3)
	O2	0.1334(14)	0	0.259(2)	0.005(3)
	O3	0.3717(12)	0	0.614(3)	0.005(3)

Table 5
Selected bonding distances (Å), angles (°) and polyhedral volumes (Å^3) for the structure of α-$ZrMo_2O_8$ at 0.20 – 0.90 GPa. Standard uncertainties (s.u.'s) are given in parenthesis. [a] -y, x-y, z [b] 1-y, 1+x-y, z [c] -x+y, -x, z [d] -x+y, 1-x, z [e] -x, -y, -z [f] 1-x, 1-y, -z [g] y, -x+y, -z [h] x-y, x -z [i] x, y, z-1

P (GPa)	0.20(3)	0.32(3)	0.42(3)	0.56(3)	0.63(3)	0.72(3)	0.80(3)	0.90(3)
$Zr1 - O1^{a,c,e,g,h}$	1.97(4)×6	1.94(4)×6	1.89(5)×6	1.90(6)×6	1.90(5)×6	1.89(6)×6	1.91(5)×6	1.94(4)×6
$Zr2^i - O2^{b,d}$	2.11(3)×3	2.12(4)×3	2.06(4)×3	2.06(6)×3	2.08(4)×3	2.09(6)×3	2.14(4)×3	2.16(3)×3
$Zr2^i - O3^{b,d}$	1.94(3)×3	1.99(3)×3	1.90(3)×3	1.88(4)×3	1.89(3)×3	1.86(3)×3	1.87(3)×3	1.91(3)×3
Mo – O1	1.92(4)	1.91(5)	1.92(5)	1.91(6)	1.90(6)	1.91(6)	1.89(5)	1.87(4)
Mo – O2	1.78(3)	1.82(4)	1.90(5)	1.90(6)	1.88(5)	1.88(7)	1.85(5)	1.85(4)
$Mo - O3^f$	1.94(4)	1.90(4)	2.01(4)	2.03(5)	2.03(5)	2.04(5)	2.05(4)	2.03(4)
Mo – O4	1.667(8)	1.681(9)	1.564(11)	1.550(13)	1.567(13)	1.563(13)	1.542(11)	1.525(11)
$O1^{a,e,g} - Zr1 - O1^{a,c,g,h}$	85(2)×6	89(2)×6	82(3)×6	81(3)×6	82(3)×6	81(3)×6	81(2)×6	82(2)×6
$O1^{a,c} - Zr1 - O1^{e,g,h}$	95(2)×6	91(2)×6	98(3)×6	99(3)×6	98(3)×6	99(3)×6	99(2)×6	98(2)×6
$O1^{a,c} - Zr1 - O1^{e,g,h}$	180(5)×3	180(3)×3	180(10)×3	180(15)×3	180(9)×3	180(16)×3	180(14)×3	180(3)×3
$O2^b - Zr2^i - O2^{b,d}$	85.8(13)×3	83(2)×3	83(2)×3	82(3)×3	81(2)×3	80(3)×3	80(2)×3	76.8(18)×3
$O2^{b,d} - Zr2^i - O3^{b,d}$	90.9(13)×3	92.4(18)×3	95(2)×3	96(3)×3	96(2)×3	97(3)×3	97(2)×3	99.5(18)
$O2^{b,d} - Zr2^i - O3^{b,d}$	175.8(12)×3	174.8(19)×3	175(2)×3	176(3)×3	176(3)×3	177(3)×3	176(2)×3	176.1(18)×3
$O2^{b,d} - Zr2^i - O3^d$	96.6(11)×3	98.9(15)×3	101(2)×3	101(2)×3	101(2)×3	101(2)×3	102(2)	103(2)×3
$O3^b - Zr2 - O3^{b,d}$	86.8(14)×3	85.9(11)×3	81.7(15)×3	81(2)×3	81(2)×3	82(2)×3	81.3(18)	80.5(17)
O1 – Mo – O2	113.5(17)	114(2)	111(2)	110(3)	111(2)	111(3)	112(2)	114(2)
$O1 - Mo - O3^f$	115.8(16)	115.0(19)	112(2)	112(3)	112(3)	111(3)	110(2)	110(2)
O1 – Mo – O4	103(2)	107.5(19)	116(2)	116(2)	114(2)	114(2)	114(2)	113(2)
$O2 - Mo - O3^f$	111.0(16)	111(2)	110(2)	111(3)	112(3)	112(4)	112(3)	114(2)
O2 – Mo – O4	109(2)	106.1(19)	106.1(19)	106(2)	106(2)	105(2)	105(2)	105.8(19)
$O3^f - Mo - O4$	103(2)	102(2)	101.6(19)	102(2)	102(2)	103(2)	102(2)	99.2(19)
Zr1 – O1 – Mo	155(2)	160.9(19)	173(3)	176(4)	175(3)	174(4)	173(4)	173(3)
Zr2 – O2 – Mo	162.8(17)	160.7(16)	160.9(17)	160(2)	158.9(16)	158(2)	156.8(15)	152.8(12)
$Zr2 - O3^f - Mo^f$	148.8(14)	146.9(10)	144.5(11)	144.2(14)	143.7(13)	145.5(13)	143.9(12)	142.5(12)
$V_{poly}(Zr1O_6)$	10.2(3)	9.8(3)	8.8(2)	8.7(3)	8.9(3)	8.8(3)	8.9(3)	9.4(2)
$V_{poly}(Zr2O_6)$	11.07(17)	11.4(2)	10.0(3)	9.9(3)	10.1(3)	9.9(3)	10.3(3)	10.7(2)
$V_{poly}(MoO_4)$	3.06(14)	3.07(8)	3.17(10)	3.17(10)	3.15(9)	3.17(11)	3.08(8)	2.99(7)

Table 6
Selected bonding distances (Å), angles (°) and polyhedral volumes (Å^3) in the structure of δ-$ZrMo_2O_8$ at 1.17 – 1.87 GPa. Standard uncertainties (s.u.'s) are given in parenthesis. ^{j} -x, y, -z ^{k} x, -y, z ^{l} x, 1-y, z ^{m} 1/2-x, -1/2+y, -z ^{n} 1/2-x, 1/2+y, -z ^{o} 1/2+x, 1/2+y, z ^{p} 1/2-x, 1/2+y, -z

P (GPa)	1.17(3)	1.48(4)	1.53(4)	1.64(4)	1.79(4)	1.87(4)
Zr^o – $O1^{e,j,l}$	2.064(16)×4	2.024(11)×4	2.026(15)×4	2.023(11)×4	2.022(11)×4	2.020(12)×4
Zr^o – $O2^j$	1.756(16)×2	1.820(12)×2	1.816(12)×2	1.834(12)×2	1.828(12)×2	1.829(12)×2
Mo – $O1^k$	1.814(17)×2	1.852(12)×2	1.848(16)×2	1.846(12)×2	1.853(12)×2	1.857(13)×2
Mo – $O2^m$	2.012(16)	1.969(14)	1.980(14)	1.934(11)	1.937(14)	1.938(14)
Mo – O3	1.530(17)	1.586(16)	1.629(16)	1.606(11)	1.608(11)	1.598(16)
$O1^e$ – Zr^o – $O1^{j,l}$	84.5(6)×2	86.1(5)×2	85.7(6)×2	86.6(4)×2	87.4(4)×2	85.8(5)×2
$O1^j$ – Zr^o – $O1^{e,l}$	95.5(6)×2	93.9(5)×2	94.3(6)×2	93.4(4)×2	92.6(4)×2	94.2(5)×2
$O1^j$ – Zr^o – $O1^{e,l}$	180(1)×2	180(2) ×2	180(2)×2	180(2)×2	180(1)×2	180(2)×2
$O1^{e,j,l}$ – Zr^o – $O2^j$	83.7(5)×4	84.8(4)×4	85.5(4)×4	85.2(4)×4	84.9(4)×4	84.0(4)×4
$O1^{e,j,l}$ – Zr^o – $O2^j$	96.5(5)×4	95.2(4)×4	94.5(4)×4	94.8(4)×4	95.1(4)×4	96.0(5)×4
O2 – Zr^o – $O2^j$	180(1)	180(3)	180(2)	180(2)	180(3)	180(2)
O1 – Mo – $O1^k$	106.8(8)	109.7(5)	109.6(6)	110.9(5)	111.8(5)	109.4(6)
$O1^k$ – Mo – $O2^m$	107.3(5)×2	104.8(4)×2	105.2(4)×2	105.3(4)×2	104.5(4)×2	104.0(4)×2
$O1^k$ – Mo – O3	112.3(6)×2	112.8(4)×2	112.6(4)×2	112.0(4)×2	112.6(4)×2	114.3(5)×2
$O2^m$ – Mo – O3	117.0(7)	111.5(6)	111.2(6)	111.0(5)	110.1(6)	109.9(6)
Zr – $O1^p$ – Mo	165.0(8)	165.0(7)	165.7(8)	165.6(6)	164.4(6)	163.6(7)
Zr – $O2^n$ – Mo^n	144.1(9)	140.9(6)	140.3(6)	140.9(6)	141.1(6)	140.8(7)
$V_{poly}(ZrO_6)$	9.79(10)	9.83(7)	9.87(8)	9.90(7)	9.86(7)	9.78(7)
$V_{poly}(MoO_4)$	2.92(4)	3.04(3)	3.10(4)	3.02(3)	3.04(3)	3.04(4)

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