SUPPLEMENTARY INFORMATION

Stable magnesium peroxide at high pressure

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Supplementary Tables

Supplementary Table S1. Lattice parameters of *I4/mcm* MgO_2

Run #	P, GPa			a, Å	σ (a, Å)	c, Å	σ (c, Å)	V, (Å3)	σ (V, $Å^3$)
	MgO		Au						
	Ref.[1]	Ref.[2]	Ref.[3]						
A1	93.5	**95.6**	-	3.9994	0.0009	4.7458	0.0032	75.9104	0.0482
A1	94.0	**96**	-	3.9988	0.0010	4.7343	0.0031	75.7028	0.0417
A1	95.5	**97.6**	-	3.9973	0.0014	4.7271	0.0034	75.5300	0.0501
A1	95.7	**97.8**	-	3.9961	0.0008	4.7243	0.0038	75.4409	0.0501
A1	97	**99.2**	-	3.99161	0.0008	4.7181	0.0031	75.1726	0.0469
A2	101.5	**104**	-	3.9787	0.0001	4.7188	0.0004	74.6971	0.0058
A2	102.5	**105**	-	3.9803	0.0001	4.7115	0.0004	74.6421	0.0058
B2	130.0	**134.3**	-	3.9211	0.0007	4.6040	0.0027	70.7882	0.0375
B2	131.5	**135.9**	-	3.92225	0.0008	4.6026	0.0027	70.8061	0.0376
B2	139.0	**144**	149,9	3.8985	0.0007	4.5605	0.0027	69.3124	0.0363
B2	154.0	**159.9**	161.1	3.8666	0.0013	4.5646	0.0038	68.2455	0.0559
B2*	152.0	**158**	156.8	3.8862	0.0009	4.5502	0.0028	68.7188	0.0362
B2*	150.0	**155.8**	152.9	3.8909	0.0014	4.5849	0.0033	69.4122	0.0458
B2*	146.5	**152.1**	151.6	3.9060	0.0008	4.5529	0.0035	69.4645	0.0535
B2*	116.5	**119.9**	116.5	3.9451	0.0010	4.6359	0.0030	72.1509	0.0450
B2*	115.0	**118.3**	-	3.9666	0.0009	4.6063	0.0028	72.4751	0.0385
B2*	114.5	**117.8**	109	3.9619	0.0010	4.6631	0.0031	73.1970	0.0459
B2*	112.0	**115.1**	111.5	3.9617	0.0013	4.6617	0.0039	73.1655	0.0612
B2*	110.0	**113**	-	3.9800	0.0010	4.6614	0.0031	73.8394	0.0463
B2*	108.0	**110.9**	-	3.9718	0.0013	4.6822	0.0040	73.8614	0.0620
B2*	103.0	**105.6**	104.8	3.9831	0.0014	4.7070	0.0040	74.6762	0.0630
B2*	83.5	**85**	-	4.0478	0.0012	4.8181	0.0034	78.9424	0.0520
B2*	83.0	**84.4**	-	4.0299	0.0014	4.8199	0.0042	78.2748	0.0676
B2*	82.5	**83.9**	-	4.0517	0.0012	4.8096	0.0034	78.9547	0.0519
B2*	74.0	**75**	74.2	4.0784	0.0019	4.8687	0.0040	80.9809	0.0585

Pressure was gauged using MgO EOS by Speziale et al. [1], Tange et al. [2], and Au EOS is after Fei et al. [3]. Pressure values used to construct *I4/mcm* MgO2 EOS are shown in bold. Decompression run is marked with an asterisk.

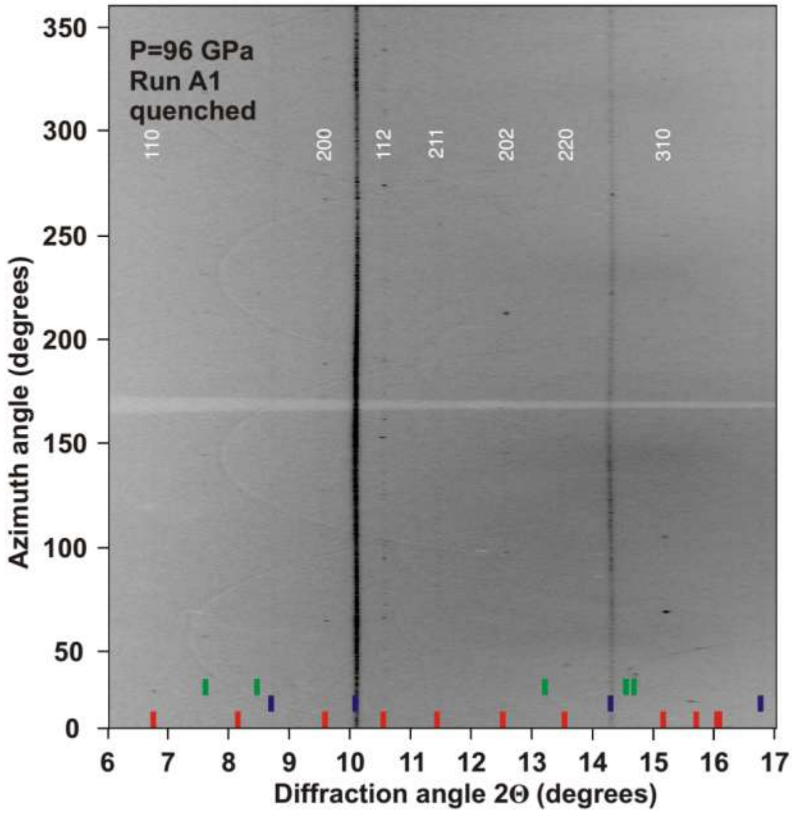
Supplementary Table S2. Computed lattice parameters of *I4/mcm* MgO_2

P, GPa	a, Å	c, Å
70	4.0853	4.8762
80	4.0572	4.8277
90	4.0315	4.7836
100	4.0076	4.7409
110	3.9855	4.7021
120	3.9649	4.6662
130	3.9455	4.6325
140	3.9272	4.6004
150	3.9101	4.5697

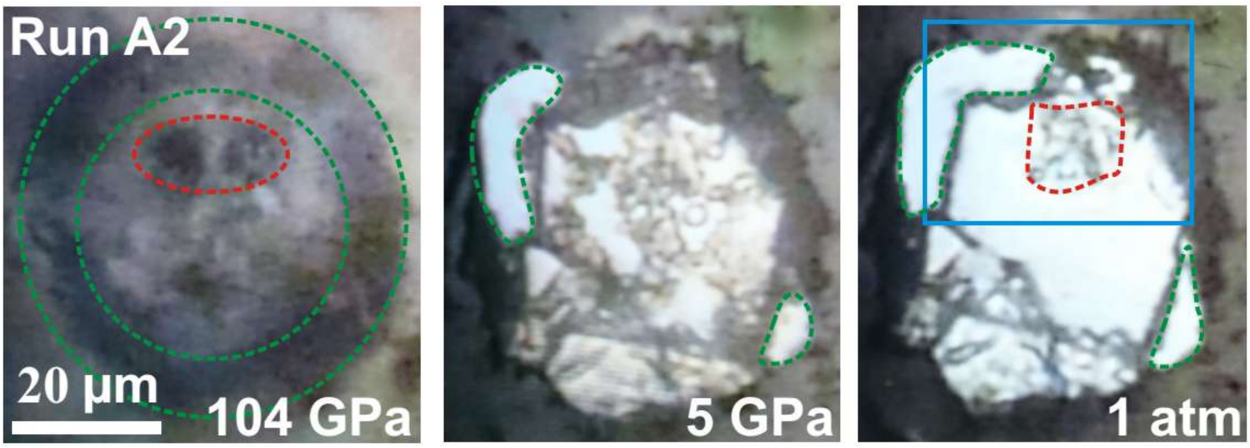
Supplementary Table S3. Experimentally and theoretically (DFT) derived parameters of the 300 K third-order Birch-Murnaghan EOS of *I4/mcm* MgO_2

	V_0, Å^3	K_0, GPa	K_0`
Compression	105.4	151.6	4
Decompression	110.1	127.1	4
DFT	106.8	147	4.1
MgO (Ref.[1])	74.71	160.2	3.99
MgO (Ref.[2])	74.698	160.64	4.221

Supplementary Figures

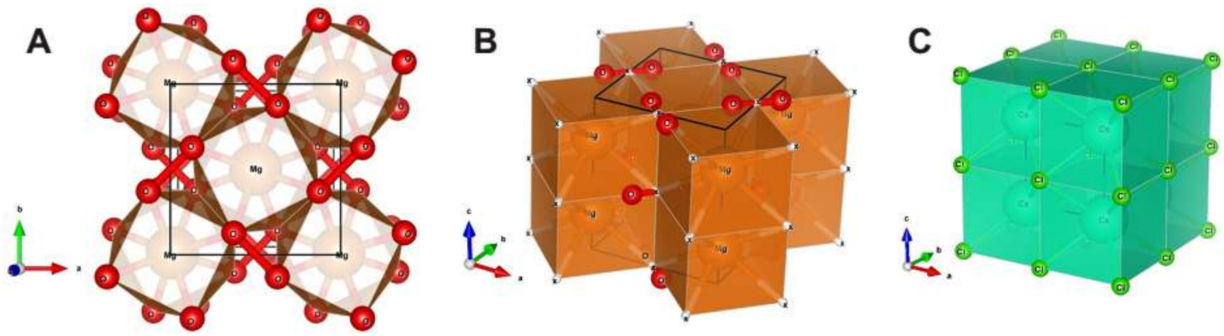


Supplementary Figure S1. *XRD image (cake) of I4/mcm MgO_2 synthesized at 96 GPa from the mixture of MgO and O_2. Red and violet ticks correspond to the positions of I4/mcm MgO_2 and MgO, respectively. Green ticks represent spotty reflections of ζ-O_2. White labels are Miller indices of the indexed tetragonal phase. A slight curvature of the vertical lines (originating from MgO is due to a pressure gradient in the sample cavity). The x-ray wavelength is 0.3344 Å.*

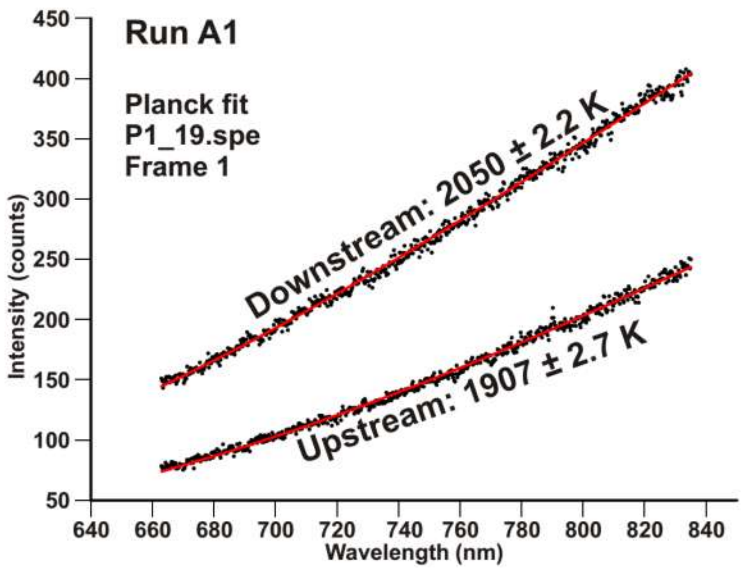


Supplementary Figure S2. *Optical images of the A2 sample in a DAC cavity. Laser-heated area (red dashed line) is shielded from Re gasket by oxygen (green dashed lines). Note the transition from the metallic ζ-O_2 at*

104 GPa (opaque) to transparent at 5 GPa. At 1 atm oxygen was no longer trapped in the DAC. Blue solid line corresponds to the sample area shown in the Figure 5.



Supplementary Figure S3. *The crystal structure of I4/mcm MgO_2 (panels **A** and **B**) as compared to CsCl-type (**C**). Lattice positions marked with an x in panel B are centers of the O-O dumbbells. Black solid lines represent unit cells. Crystal structures were visualized by S.S.L. using VESTA v.3 (Ref.[4]).*



Supplementary Figure S4. *Planck fits (red curves) to the collected thermal radiation (black dots). Only statistical uncertainty related to the fit quality is shown.*

Supplementary References

1. *Speziale, S., Zha, C. S., Duffy, T. S., Hemley, R. J., Mao, H. K. Quasi-hydrostatic compression of magnesium oxide to 52 GPa: Implications for the pressure-volume-temperature equation of state. Journal of Geophysical Research,* ***106,*** *515-528 (2001).*

2. *Tange, Y., Nishihara, Y., Tsuchiya, T. Unified analyses for P-V-T equation of state of MgO: A solution for pressure-scale problems in high P-T experiments. J Geophys Res-Sol Ea,* ***114,*** *(2009).*

3. *Fei, Y. W., et al. Toward an internally consistent pressure scale. Proc. Natl. Acad. Sci. U.S.A.,* ***104,*** *9182-9186 (2007).*

4. *Momma, K. & Izumi, F. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. J. Appl. Crystallogr.,* ***44,*** *1272-1276 (2011).*