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**Supporting information for article:**

**Structure evolution of  $\text{Bi}_4\text{O}_7$  under high pressure**

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**Table S1:** Lattice parameters for Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi <sub>4</sub> O <sub>7</sub>	0 MPa	3800 MPa	9700 MPa	10400 MPa
$V [\text{Å}^3]$	340.39	333.39 [97.9 %]	311.29 [91.5 %]	308.34 [90.6 %]
$a [\text{Å}]$	6.7253	6.6715 [99.2 %]	6.4867 [96.5 %]	6.4558 [96.0 %]
$b [\text{Å}]$	6.9950	6.9419 [99.2 %]	6.7725 [96.8 %]	6.7522 [96.5 %]
$c [\text{Å}]$	7.7961	7.7635 [99.6 %]	7.6336 [97.9 %]	7.6213 [97.8 %]
$\alpha [^\circ]$	72.556	72.4436	71.9669	71.947
$\beta [^\circ]$	88.842	89.9260	88.8797	88.859
$\gamma [^\circ]$	76.925	77.1581	77.7930	77.782

**Table S2:** BiO<sub>n</sub> polyhedral volume and Bi-O distances for Bi1 in Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi1	0 MPa	3800 MPa	9700 MPa	10400 MPa
V [Å <sup>3</sup> ]	29.289	28.687	26.785	26.531
		[97.9 %]	[91.5 %]	[90.6 %]
O4 [Å]	2.160	2.140	2.075	2.066
		[99.1 %]	[96.1 %]	[95.6 %]
O7 [Å]	2.249	2.255	2.202	2.196
		[100.3 %]	[97.9 %]	[97.6 %]
O4 [Å]	2.274	2.240	2.215	2.209
		[98.5 %]	[97.4 %]	[97.1 %]
O3 [Å]	2.633	2.609	2.557	2.548
		[99.1 %]	[97.1 %]	[96.8 %]
O1 [Å]	2.662	2.628	2.595	2.590
		[98.7 %]	[97.5 %]	[97.3 %]
O2 [Å]	2.719	2.723	2.666	2.660
		[100.1 %]	[98.1 %]	[97.8 %]
O5 [Å]	2.954	2.929	2.851	2.842
		[99.2 %]	[96.5 %]	[96.2 %]
O2 [Å]	3.164	3.134	3.040	3.027
		[99.1 %]	[96.1 %]	[95.7 %]

**Table S3:** BiO<sub>n</sub> polyhedral volume and Bi-O distances for Bi2 in Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi2	0 MPa	3800 MPa	9700 MPa	10400 MPa
V [Å <sup>3</sup> ]	23.692	23.205	21.667	21.461
		[97.9 %]	[91.5 %]	[90.6 %]
O2 [Å]	2.079	2.051	2.024	2.019
		[98.7 %]	[97.4 %]	[97.1 %]
O1 [Å]	2.182	2.184	2.139	2.133
		[100.1 %]	[98.0 %]	[97.8 %]
O7 [Å]	2.225	2.212	2.135	2.126
		[99.4 %]	[96.0 %]	[95.6 %]
O7 [Å]	2.670	2.632	2.604	2.597
		[98.6 %]	[97.5 %]	[97.3 %]
O4 [Å]	2.723	2.731	2.668	2.661
		[100.3 %]	[98.0 %]	[97.7 %]
O1 [Å]	2.995	2.976	2.875	2.862
		[99.4 %]	[96.0 %]	[95.6 %]
O6 [Å]	3.024	2.999	2.924	2.915
		[99.2 %]	[96.7 %]	[96.4 %]

**Table S4:** BiO<sub>n</sub> polyhedral volume and Bi-O distances for Bi4 in Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi4	0 MPa	3800 MPa	9700 MPa	10400 MPa
V [Å <sup>3</sup> ]	21.368	20.929	19.541	19.356
		[97.9 %]	[91.4 %]	[90.6 %]
O5 [Å]	2.198	2.163	2.139	2.133
		[98.4 %]	[97.3 %]	[97.0 %]
O6 [Å]	2.213	2.221	2.157	2.150
		[100.4 %]	[97.5 %]	[97.2 %]
O4 [Å]	2.277	2.257	2.200	2.193
		[99.1 %]	[96.6 %]	[96.3 %]
O7 [Å]	2.405	2.385	2.324	2.317
		[99.2 %]	[96.6 %]	[96.3 %]
O5 [Å]	2.530	2.539	2.474	2.468
		[100.4 %]	[97.8 %]	[97.5 %]
O6 [Å]	2.733	2.697	2.666	2.660
		[98.7 %]	[97.5 %]	[97.3 %]
O3 [Å]	2.761	2.739	2.655	2.643
		[99.2 %]	[96.2 %]	[95.7 %]

**Table S5:** BiO<sub>6</sub> octahedral volume and Bi-O distances for Bi3 in Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi3	0 MPa	3800 MPa	9700 MPa	10400 MPa
V [Å <sup>3</sup> ]	11.826	11.582	10.815	10.712
		[97.9 %]	[91.5 %]	[90.6 %]
O6 [Å]	2.021	2.012	1.946	1.937
		[99.6 %]	[96.3 %]	[95.8 %]
O6 [Å]	2.021	2.012	1.946	1.937
O1 [Å]	2.093	2.077	2.033	2.027
		[99.2 %]	[97.1 %]	[96.8 %]
O1 [Å]	2.093	2.077	2.033	2.027
O3 [Å]	2.126	2.103	2.076	2.072
		[98.9 %]	[97.6 %]	[97.5 %]
O3 [Å]	2.126	2.103	2.076	2.072
min. O-Bi-O [°]	81.79	82.24	82.20	82.24
max. O-Bi-O [°]	98.21	97.76	97.80	97.76

**Table S6:** BiO<sub>6</sub> octahedral volume and Bi-O distances for Bi5 in Bi<sub>4</sub>O<sub>7</sub> at ambient pressure [39] and upon applying high pressure. The relative size referring to the value at ambient pressure is written in square brackets.

Bi5	0 MPa	3800 MPa	9700 MPa	10400 MPa
V [Å <sup>3</sup> ]	12.458	12.202	11.393	11.285
		[97.9 %]	[91.5 %]	[90.6 %]
O3 [Å]	2.091	2.093	2.050	2.045
		[100.1 %]	[98.0 %]	[97.8 %]
O3 [Å]	2.091	2.093	2.050	2.045
O5 [Å]	2.117	2.095	2.037	2.028
		[99.0 %]	[96.2 %]	[95.8 %]
O5 [Å]	2.117	2.095	2.037	2.028
O2 [Å]	2.136	2.115	2.070	2.064
		[99.0 %]	[96.9 %]	[96.6 %]
O2 [Å]	2.136	2.115	2.070	2.064
min. O-Bi-O [°]	83.09	82.94	82.80	82.86
max. O-Bi-O [°]	96.91	97.06	97.20	97.14