Supplemental Material to the article

"Stability of defect-free structures of titanium monoxide at high pressures"

# in ascending order of the ground state energy	Parameters of the primitive cell generated by the code USPEX	Coordinates of atoms in a primitive cell
1	$a = b = 498$ pm, $c = 285$ pm, $\alpha = \beta = 90°$, $\gamma = 120°$	Ti1 (0, 0, 0), Ti2 (0.333, 0.667, 0.5), Ti3 (0.667, 0.333, 0.5), O1 (0.394, 1, 0), O2 (0.606, 0.606, 0), O3 (1, 0.394, 0)
2	$a = 507$ pm, $b = 579$ pm, $c = 414$ pm, $\alpha = 90°$, $\beta = 65.9°$, $\gamma = 105.8°$	Ti1 (0.386, 0.426, 0.156), Ti2 (0, 0.580, 0.843), Ti3 (0, 0, 0.83), Ti4 (0.710, 0.753, 0.5), Ti5 (0, 0.580, 0.843) O1 (0, 0, 0.333), O2 (0.369, 0.420, 0.667), O3 (0.710, 0.25, 1), O4 (0, 0.60, 0.333), O5 (0.333, 0.913, 0.667)
3	$a = 883$ pm, $b = 414$ pm, $c = 579$ pm, $\alpha = \beta = \gamma = 90°$	Ti1 (0.859, 0.76, 0), Ti2 (0.204, 0.76, 0), Ti3 (0.356, 0.26, 0.286), Ti4 (0.706, 0.260, 0.278), Ti5 (0.554, 0.759, 0), Ti6 (0, 0.25, 0.285), Ti7 (0, 0.25, 0.789), Ti8 (0.868, 0.760, 0.529), Ti9 (0.542, 0.760, 0.530), Ti10 (0.368, 0.25, 0.785), O1 (0.205, 0.26, 0.54), O2 (0.377, 0.76, 0.276), O3 (0.537, 0.260, 0.529), O4 (0.874, 0.26, 0.531), O5 (0, 0.76, 0.787), O6 (0.706, 0.76, 0.776), O7 (0.374, 0.76, 0.786), O8 (0.534, 0.23, 0), O9 (0.874, 0.25, 0), O10 (0, 0.76, 0.282)
4	$a = 494$ pm, $b = 571$ pm, $c = 575$ pm, $\alpha = \beta = \gamma = 90°$	Ti1 (0.387, 0.559, 0.26), Ti2 (0.886, 0.309, 0), Ti3 (0.372, 0.309, 0.76), Ti4 (0.885, 0.309, 0.51), Ti5 (0.387, 0, 0.26), Ti6 (0.886, 0.809, 0), Ti7 (0.372, 0.809, 0.76), Ti8 (0.885, 0.809, 0.51), O1 (0.78, 0.56, 0.261), O2 (0.189, 0, 0.972), O3 (0.189, 0.559, 0.549), O4 (0.189, 0, 0.549), O5 (0.704, 0.559, 0.76), O6 (0.189, 0.559, 0.971), O7 (0.780, 0, 0.26), O8 (0.7, 0, 0.761)
5	$a = c = 582$ pm, $b = 284$ pm, $\alpha = 76.07°$, $\beta = 71.05°$, $\gamma = 103.92°$	Ti1 (0.351, 0.258, 0), Ti2 (0.312, 0.966, 0.572), Ti3 (0.809, 0.966, 0), Ti4 (0.77, 0.675, 0.61), O1 (1, 0.25, 0.67), O2 (0.41, 0.675, 0.25), O3 (0.71, 0.25, 0.382), O4 (0.122, 0.674, 0.971)
6	$a = 868$ pm, $b = 765$ pm, $c = 285$ pm, $\alpha = \beta = 90°$, $\gamma = 100.7°$	Ti1 (0.21, 0, 0.519), Ti2 (0.429, 0.333, 0.519), Ti3 (0, 0.333, 0.521), Ti4 (0.532, 0, 0.52), Ti5 (0.647, 0.67, 0.519), Ti6 (0.986, 0.672, 0.52), Ti7 (0.759, 0.346, 0), Ti8 (0.317, 0.665, 0), Ti9 (0.87, 0.986, 0), O1 (0.548, 0.208, 0), O2 (0.242, 0.227, 0), O3 (0.94, 0.236, 0), O4 (0.648, 0.873, 0), O5 (0.806, 0.607, 0), O6 (0, 0.87, 0), O7 (0.1, 0.539, 0), O8 (0.357, 0.924, 0), O9 (0.49, 0.535, 0)

# in ascending order of the ground state energy	Parameters of the primitive cell generated by the code USPEX	Coordinates of atoms in a primitive cell
7	$a = 773\,\text{pm}$, $b = 581\,\text{pm}$, $= 572\,\text{pm}$, $\alpha = 60.5°$, $\beta = 90°$, $\gamma = 73.4°$	Ti1 (0.373, 0.635, 0.109),Ti2 (0.558, 0, 0.15), Ti3 (0.987, 0.839, 0.25), Ti4 (0.373, 0.635, 0.609), Ti5 (0.773, 0.454, 0.200), Ti6 (0.773, 0.455, 0.7), Ti7 (0.172, 0.236, 0.308), Ti8 (0.987, 0.839, 0.757), Ti9 (0.558, 0, 0.65), Ti10 (0.172, 0.236, 0.808), O1 (0.973, 0.231, 0.561), O2 (0.331, 0.956, 0.698), O3 (0.214, 0.516, 0.918), O4 (0.331, 0.956, 0.198), O5 (0.214, 0.516, 0.418), O6 (0.573, 0.431, 0.961), O7 (0.573, 0.431, 0.461), O8 (0.973, 0.231, 0), O9 (0.773, 0.731, 0.311), O10 (0.772, 0.732, 0.812)
8	$a = 295\,\text{pm}$, $b = 538\,\text{pm}$, $c = 609\,\text{pm}$, $\alpha = 102.5°$, $\beta = 104°$, $\gamma = 74.1°$	Ti1 (0.141, 0.203, 0.455), Ti2 (0.565, 1, 0), Ti3 (0.92, 0.77, 0.583), Ti4 (0.344, 0.536, 0.191), O1 (0.360, 0, 0.715), O2 (0.542, 0.484, 0.54), O3 (0.943, 0.25, 0.1), O4 (0.125, 0.716, 0.932)
9	$a = b = 411\,\text{pm}$, $c = 105\,\text{pm}$, $\alpha = 78.9$, $\beta = \gamma = 90°$	Ti1 (0.615, 0.862, 0.25), Ti2 (0.115, 0.364, 0.25057), Ti3 (0.116, 0.758, 0.453), Ti4 (0.618, 0, 0.863), Ti5 (0.118, 0.549, 0.862), Ti6 (0.118, 0.162, 0.639), Ti7 (0.618, 0.659, 0.64), Ti8 (0.617, 0.46, 0), O1 (0.115, 0.865, 0.249), O2 (0.615, 0.362, 0.253), O3 (0.118, 0, 0.843), O4 (0.616, 0.957, 0), O5 (0.616, 0.761, 0.448), O6 (0.116, 0.261, 0.448), O7 (0.618, 0.15, 0.659, O8 (0.116, 0.458, 0)
10	$a = 583\,\text{pm}$, $b = 771\,\text{pm}$, $c = 584\,\text{pm}$, $\alpha = 78.7°$, $\beta = 60.6°$, $\gamma = 100.8°$	Ti1 (0.883, 0.25, 0.85), Ti2 (0.351, 0.899, 0.195), Ti3 (0.363, 0.569, 0.538), Ti4 (0.365, 0.233, 0.86), Ti5 (0.361, 0.567, 0), Ti6 (0.357, 0.216, 0.357), Ti7 (0.876, 0.234, 0.347), Ti8 (0.889, 0.568, 0), Ti9 (0.877, 0.897, 0.67), Ti10 (0.879, 0.9, 0.196), O1 (0.614, 0.398, 0.432), O2 (0.12, 0.733, 0.604), O3 (0.627, 0, 0.774), O4 (0.111, 0, 0.774), O5 (0.621, 0.405, 0.941), O6 (0.62, 0.733, 0.604), O7 (0.619, 0, 0.267), O8 (0.129, 0.404, 0.434), O9 (0.62, 0.733, 0.104), O10 (0.12, 0.733, 0.104)
11	$a = 514\,\text{pm}$, $b = 509\,\text{pm}$, $c = 507\,\text{pm}$, $\alpha = 99.4°$, $\beta = 79.1°$, $\beta = 80°$	Ti1 (0.603, 0.276, 0.463), Ti2 (0.185, 0.139, 0.111), Ti3 (0, 0.431, 0.723), Ti4 (0.736, 0.985, 0.852), Ti5 (0.465, 0.558, 0), Ti6 (0.322, 0.856, 0.563), O1 (0.109, 0.784, 0.931), O2 (0.817, 0.34, 0), O3 (0.252, 0.483, 0.358), O4 (0.677, 0.632, 0.643), O5 (0.534, 0.931, 0.216), O6 (0.97, 0, 0.502)
12	$a = 618\,\text{pm}$, $b = 296\,\text{pm}$, $c = 525\,\text{pm}$, $\alpha = 106.3°$, $\beta = 102.8°$, $\gamma = 76.3°$	Ti1 (0.529, 0.465, 0.693), Ti2 (0.387, 0.252, 0.12), Ti3 (0.134, 0, 0.464), Ti4 (0.993, 0.834, 0.892), O1 (0.476, 0.848, 0.403), O2 (0.654, 0, 0.952), O3 (0.867, 0.269, 0.633), O4 (0, 0.451, 0.181)
13	$a = 604\,\text{pm}$, $b = 287\,\text{pm}$, $c = 581\,\text{pm}$, $\alpha = 75.8°$, $\beta = 63.3o$, $\gamma = 90.4°$	Ti1 (0.683, 0.646, 0.384), Ti2 (0.673, 0.376, 0.924), Ti3 (0.110, 0.15, 0.383), Ti4 (0.1, 0.879, 0.923), O1 (0.306, 0.348, 0.984), O2 (0.477, 0.177, 0.323), O3 (0.72, 0, 0.62), O4 (0, 0.498, 0.687)
14	$a = 580\,\text{pm}$, $b = 667\,\text{pm}$, $c = 493\,\text{pm}$, $\alpha = 94°$, $\beta = 90°$, $\gamma = 64.3°$	Ti1 (0.582, 0.588, 0.729, Ti2 (0, 0.588, 0.729), Ti3 (0.546, 0.161, 0.718), Ti4 (0.418, 0.415, 0.268), Ti5 (0.918, 0.415, 0.268), Ti6 (0.455, 0.842, 0.279), Ti7 (0.955, 0.842, 0.279), Ti8 (0, 0.161, 0.718), O1 (0.719, 0.314, 0.958), O2 (0.781, 0.689, 0), O3 (0.414, 0.924, 0.691), O4 (0.587, 0, 0.306), O5 (0.282, 0.689, 0), O6 (0.219, 0.314, 0.959), O7 (0, 0, 0.306), O8 (0.914, 0.924, 0.691)
15	$a = 625\,\text{pm}$, $b = 588\,\text{pm}$, $c = 384\,\text{pm}$, $\alpha = \beta = \gamma = 90°$	Ti1 (0.503, 0.25, 0), Ti2 (0.494, 0.752, 0), Ti3 (0.77, 0, 0.623), Ti4 (0.227, 1, 0.627), Ti5 (0.77, 0.496, 0.623), Ti6 (0.226, 0.507, 0.627), O1 (0.726, 0.995, 0.13), O2 (0.271, 0, 0.132), O3 (0.726, 0.509, 0.13), O4 (0.27, 0.495, 0.133), O5 (1, 0.25, 0.63), O6 (1, 0.752, 0.63)

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16	$a = 293\,\text{pm}$, $b = 384\,\text{pm}$, $c = 626\,\text{pm}$, $\alpha = \beta = \gamma = 90^\circ$	Ti1 (0.778, 0.208, 0.343), Ti2 (0.778, 0.207, 0.887), Ti3 (0.275, 0.751, 0.615), O1 (0.772, 0.702, 0.387), O2 (0.277, 0.201, 0.115), O3 (0.774, 0.7, 0.844)
17	$a = 293\,\text{pm}$, $b = 384\,\text{pm}$, $c = 625\,\text{pm}$, $\alpha = \beta = \gamma = 90^\circ$	Ti1 (0.274, 0.536, 0.613), Ti2 (0.775, 0, 0.885), Ti3 (0.775, 0, 0.341), O1 (0.775, 0.583, 0.385), O2 (0.275, 0, 0.113), O3 (0.774, 0.595, 0.841)
18	$a = 587\,\text{pm}$, $b = 776\,\text{pm}$, $c = 574\,\text{pm}$, $\alpha = 111.2^\circ$, $\beta = 60.8^\circ$, $\gamma = 100.3^\circ$	Ti1 (0.734, 0.23, 0.359), Ti2 (0.57, 0.892, 0.532), Ti3 (0.893, 0.552, 0.189), Ti4 (0.218, 0.241, 0.875), Ti5 (0.384, 0.569, 0.189), Ti6 (0.736, 0.22, 0.847), Ti7 (0.221, 0.231, 0.363), Ti8 (0.889, 0.565, 0.69), Ti9 (0, 0.91, 0.532), Ti10 (0, 0.897, 0), O1 (0, 0.404, 0.771), O2 (0.745, 0.731, 0.595), O3 (0.397, 0, 0.455), O4 (0.398, 0, 0.942), O5 (0.557, 0.396, 0.272), O6 (0.209, 0.731, 0.126), O7 (0.887, 0, 0.95), O8 (0.556, 0.4, 0.78), O9 (0.727, 0.734, 0.114), O10 (0.227, 0.728, 0.607)
19	$a = 502\,\text{pm}$, $b = 411\,\text{pm}$, $c = 1046\,\text{pm}$, $\alpha = 101.2^\circ$, $\beta = 93.6^\circ$, $\gamma = 114.1^\circ$	Ti1 (0, 0.52, 0.27), Ti2 (0.313, 0.242, 0.448), Ti3 (0.859, 0.698, 0.817), Ti4 (0.484, 0, 0.904), Ti5 (0.12, 0.418, 1), Ti6 (0.788, 0.8, 0), Ti7 (0.596, 1, 0.638), Ti8 (1, 0.61, 0.543), Ti9 (0.424, 0.164, 0.183), O1 (0.869, 0.2, 0.813), O2 (0.22, 0.832, 0.722), O3 (0.688, 0.388, 0.365), O4 (0.579, 0.467, 0.634), O5 (0.954, 0.11, 0.544), O6 (0.418, 0.659, 0.179), O7 (0.329, 0.753, 0.452), O8 (0, 0, 0.274), O9 (0.489, 0.558, 0.908)
20	$a = 579\,\text{pm}$, $b = 286\,\text{pm}$, $c = 496\,\text{pm}$, $\alpha = \beta = \gamma = 90^\circ$	Ti1 (0, 0.454, 0.839), Ti2 (0.515, 0.955, 0.81), Ti3 (0.25, 0.455, 0.34), Ti4 (0.752, 0.957, 0.31), O1 (0.71, 0.456, 0.629), O2 (0, 0.955, 0.521), O3 (0.21, 0.954, 0), O4 (0.558, 0.457, 0.129)
21	$a = 919\,\text{pm}$, $b = 413\,\text{pm}$, $c = 583\,\text{pm}$, $\alpha = \beta = 90^\circ$, $\gamma = 71.7^\circ$	Ti1 (0.417, 1, 0.108), Ti2 (0.405, 1, 0.625), Ti3 (0, 1, 0.782), Ti4 (0.919, 0.465, 0.11), Ti5 (0.768, 0.964, 0.434), Ti6 (0.578, 0.464, 0.25), Ti7 (0.92, 0.465, 0.612), Ti8 (0.578, 0.464, 0.807), Ti9 (0.242, 0.463, 0.447), Ti10 (0.244, 0.463, 0.95), O1 (0.916, 1, 0.107), O2 (0, 0.464, 0.28), O3 (0.583, 1, 0.29), O4 (0.422, 0.471, 0.606), O5 (0.918, 0.965, 0.614), O6 (0.588, 1, 0.767), O7 (0.753, 0.465, 0.944), O8 (0.238, 1, 1), O9 (0.745, 0.464, 0.448), O10 (0.243, 1, 0.44)
22	$a = 868\,\text{pm}$, $b = 880\,\text{pm}$, $c = 286\,\text{pm}$, $\alpha = \beta = 90^\circ$, $\beta = 119.4^\circ$	Ti1 (0.357, 0, 0), Ti2 (0.36, 0.354, 0.517), Ti3 (0, 0.336, 0.518), Ti4 (0.68, 0, 0.517), Ti5 (0.685, 0.676, 0.518), Ti6 (0, 0.665, 0.518), Ti7 (0.681, 0.345, 0), Ti8 (0.342, 0.667, 0), Ti9 (0, 0, 0), O1 (0.494, 0.918, 0), O2 (0.144, 0.278, 0), O3 (0.806, 0.207, 0), O4 (0.758, 0.875, 0), O5 (0.806, 0.598, 0), O6 (0.108, 0.842, 0), O7 (0, 0.536, 0), O8 (0.231, 0, 0.515), O9 (0.482, 0.547, 0)
23	$a = 582\,\text{pm}$, $b = 531\,\text{pm}$, $c = 493\,\text{pm}$, $\alpha = 97.8^\circ$, $\beta = 90^\circ$, $\gamma = 105.6^\circ$	Ti1 (0.427, 0.322, 0.531), Ti2 (0, 0.776, 0.982), Ti3 (0.926, 0.327, 0.513), Ti4 (0.289, 0.786, 0.435), Ti5 (0.664, 0.305, 0), Ti6 (0.795, 0.787, 0.431), Ti7 (0.187, 0.329, 0), O1 (0.106, 0, 0.653), O2 (0.346, 0, 0.167), O3 (0.878, 0, 0.158), O4 (0.492, 0.573, 0.23), O5 (0.615, 0, 0.633), O6 (0.237, 0.571, 0.739), O7 (0.736, 0.568, 0.742)
24	$a = 584\,\text{pm}$, $b = 511\,\text{pm}$, $c = 511\,\text{pm}$, $\alpha = 109.3^\circ$, $\beta = \gamma = 90^\circ$	Ti1 (0.518, 0.843, 0), Ti2 (0, 0.824, 0), Ti3 (0, 0.347, 0.497), Ti4 (0.264, 0.835, 0.486), Ti5 (0.772, 0.358, 0), Ti6 (0.772, 0.835, 0.487), Ti7 (0.264, 0.357, 0), O1 (0, 0, 0.759), O2 (0.764, 0.593, 0.7432), O3 (0.272, 0.593, 0.744), O4 (0.518, 0, 0.754), O5 (0.518, 0.588, 0.256), O6 (0.764, 0.1, 0.251), O7 (0.272, 0.1, 0.251)

# in ascending order of the ground state energy	Parameters of the primitive cell generated by the code USPEX	Coordinates of atoms in a primitive cell
25	$a = 771\,\text{pm}$, $b = 512\,\text{pm}$, $c = 415\,\text{pm}$, $\alpha = 66°$, $\beta = 74.7°$, $\gamma = 90°$	Ti1 (0.894, 0.249, 0.273), Ti2 (0.532, 0.346, 0.403), Ti3 (0.136, 0.513, 0.521), Ti4 (0.269, 0.109, 0.161), Ti5 (0.654, 0, 0), Ti6 (0.774, 0.643, 0.635), Ti7 (0.403, 0.785, 0.747), O1 (0.516, 0.39, 0.888), O2 (0.897, 0.25, 0.77), O3 (0.261, 0.136, 0.65), O4 (0.777, 0.634, 0.138), O5 (0.152, 0.5, 0), O6 (0.402, 0.731, 0.275), O7 (0, 0.883, 0.4)
26	$a = 584\,\text{pm}$, $b = 513\,\text{pm}$, $c = 509\,\text{pm}$, $\alpha = 80.5°$, $\beta = 89.2°$, $\gamma = 105.6°$	Ti1 (0.286, 0.703, 0.648), Ti (0.123, 0.19, 0.372), Ti3 (0.896, 0.188, 0.907), Ti4 (0.772, 0.713, 0.643), Ti5 (0.41, 0.158, 0.894), Ti6 (0.532, 0.703, 0.136), Ti7 (0.663, 0.185, 0.408), O1 (0.223, 0.441, 0), O2 (0, 0.951, 0.761), O3 (0.336, 0.946, 0.273), O4 (0.455, 0.433, 0.522), O5 (0.843, 0.92, 0.256), O6 (0.966, 0.448, 0.532), O7 (0.702, 0.436, 0)
27	$a = b = 282\,\text{pm}$, $c = 283\,\text{pm}$, $\alpha = \beta = 90°$, $\gamma = 120°$	O1 (0, 0, 0), Ti1 (0.667, 0.333, 0.5)