

Supplementary table. Unit cell parameters of CaCO₃-*Pmmn* at different *P-T* conditions.

<i>T</i> (K)	<i>P</i> (GPa)	<i>V</i> (Å ³)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)
298	49.9(1) ^a	77.55(7)	4.182(5)	4.600(6)	4.031(4)
298	52.2(1)	76.89(2)	4.155(2)	4.611(2)	4.014(5)
298	55.4(1)	76.23(6)	4.132(4)	4.594(5)	4.016(9)
298	56.1(2)	75.99(7)	4.127(5)	4.589(5)	4.013(9)
298	56.8(2)	75.77(9)	4.121(7)	4.589(7)	4.008(9)
298	59.1(2)	75.22(9)	4.104(6)	4.574(7)	4.007(9)
298	60.6(2)	74.95(7)	4.102(5)	4.576(6)	3.994(9)
298	66.1(2)	73.70(4)	4.075(3)	4.558(3)	3.967(9)
298	67.5(3)	73.36(3)	4.066(2)	4.548(2)	3.968(6)
1308(100)	60.3(5)	76.36(6)	4.144(4)	4.595(5)	4.010(9)
1317(100)	60.1(5)	76.35(4)	4.145(3)	4.597(3)	4.007(9)
1319(100)	72.3(7)	73.63(4)	4.076(2)	4.554(3)	3.967(9)
1320(100)	61.6(5)	76.17(5)	4.135(4)	4.592(4)	4.012(9)
1322(100)	72.6(6)	73.58(3)	4.073(2)	4.553(3)	3.967(9)
1326(100)	60.8(5)	76.30(7)	4.143(5)	4.597(6)	4.007(9)
1340(100)	73.1(6)	73.57(3)	4.073(2)	4.552(2)	3.968(9)
1348(100)	64.0(6)	75.62(8)	4.117(5)	4.578(6)	4.013(9)
1353(100)	64.0(5)	75.67(8)	4.118(5)	4.578(6)	4.015(9)
1354(100)	63.8(5)	75.72(9)	4.119(6)	4.578(7)	4.015(9)
1358(100)	73.3(6)	73.57(5)	4.072(4)	4.552(4)	3.970(9)
1360(100)	57.8(5)	77.04(5)	4.155(3)	4.606(4)	4.025(9)
1360(100)	57.4(5)	77.11(4)	4.158(3)	4.607(3)	4.026(9)
1360(100)	61.3(5)	76.22(4)	4.140(3)	4.594(3)	4.007(9)
1362(100)	69.2(6)	74.41(1)	4.103(1)	4.564(1)	3.974(3)
1366(100)	69.4(6)	74.28(2)	4.102(1)	4.565(2)	3.967(4)
1366(100)	69.0(6)	74.40(6)	4.103(1)	4.565(1)	3.972(5)
1368(100)	72.6(7)	73.60(2)	4.075(2)	4.554(2)	3.966(9)
1369(100)	60.1(5)	76.45(6)	4.147(4)	4.597(4)	4.010(9)
1369(100)	64.1(6)	75.61(8)	4.117(5)	4.577(6)	4.013(9)
1372(100)	63.6(5)	75.74(7)	4.119(5)	4.578(6)	4.016(9)
1374(100)	58.2(5)	76.96(5)	4.155(3)	4.605(4)	4.022(9)
1378(100)	64.6(6)	75.50(8)	4.115(6)	4.577(6)	4.009(9)
1381(100)	64.5(6)	75.60(8)	4.115(5)	4.576(6)	4.015(9)
1392(100)	64.5(6)	75.61(8)	4.116(6)	4.577(6)	4.013(9)
1393(100)	69.7(6)	74.22(4)	4.100(3)	4.565(3)	3.965(8)
1396(100)	72.5(7)	73.65(2)	4.076(2)	4.554(2)	3.968(9)
1402(100)	69.0(6)	74.49(3)	4.104(1)	4.565(2)	3.976(6)
1405(100)	69.9(6)	74.18(3)	4.100(2)	4.565(3)	3.963(7)
1414(100)	64.9(6)	75.51(8)	4.113(6)	4.576(6)	4.012(9)
1415(100)	58.8(5)	76.90(4)	4.154(3)	4.605(3)	4.021(9)
1422(100)	65.1(6)	75.51(9)	4.113(6)	4.575(7)	4.013(9)
1429(100)	59.5(5)	76.79(4)	4.151(3)	4.603(3)	4.019(8)

1430(100)	65.8(6)	75.40(9)	4.109(7)	4.574(7)	4.011(9)
1431(100)	72.8(7)	73.64(2)	4.077(1)	4.554(1)	3.967(3)
1438(100)	62.0(5)	76.24(5)	4.139(4)	4.593(4)	4.011(9)
1440(100)	70.3(6)	74.13(3)	4.100(2)	4.565(2)	3.961(6)
1445(100)	70.3(6)	74.10(2)	4.098(1)	4.564(2)	3.962(4)
1448(100)	73.9(6)	73.53(5)	4.071(3)	4.552(4)	3.968(9)
1456(100)	57.5(5)	77.17(4)	4.163(3)	4.609(3)	4.022(8)
1463(100)	72.8(7)	73.69(2)	4.079(1)	4.554(1)	3.967(4)
1467(100)	70.6(6)	74.15(2)	4.098(1)	4.564(1)	3.965(3)
1467(100)	69.3(6)	74.55(1)	4.105(1)	4.565(1)	3.979(3)
1471(100)	55.3(5)	78.42(4)	4.199(3)	4.619(3)	4.044(9)
1472(100)	60.6(5)	76.53(5)	4.147(3)	4.596(4)	4.015(9)
1479(100)	59.4(5)	76.85(4)	4.152(3)	4.604(3)	4.020(7)
1485(100)	56.9(6)	77.98(6)	4.185(4)	4.616(4)	4.036(9)
1485(100)	69.5(6)	74.55(4)	4.105(1)	4.565(3)	3.979(7)
1489(100)	69.5(6)	74.48(3)	4.104(1)	4.565(3)	3.975(3)
1490(100)	65.9(6)	75.37(7)	4.111(5)	4.576(6)	4.007(9)
1492(100)	57.3(5)	77.26(5)	4.164(3)	4.609(3)	4.025(9)
1492(100)	64.3(6)	75.79(7)	4.122(5)	4.579(5)	4.016(9)
1495(100)	54.6(5)	78.49(3)	4.200(2)	4.619(2)	4.046(6)
1500(100)	56.4(5)	78.24(3)	4.193(2)	4.616(3)	4.042(7)
1506(100)	64.5(6)	75.75(7)	4.121(5)	4.579(5)	4.014(9)
1507(100)	62.9(5)	76.18(6)	4.134(4)	4.591(5)	4.014(9)
1509(100)	65.9(6)	75.49(9)	4.112(7)	4.575(7)	4.013(9)
1511(100)	64.6(6)	75.74(7)	4.121(4)	4.579(5)	4.013(9)
1516(100)	66.2(6)	75.48(9)	4.111(7)	4.575(8)	4.014(9)
1521(100)	69.4(6)	74.65(4)	4.105(1)	4.566(3)	3.984(8)
1522(100)	62.9(5)	76.20(7)	4.136(5)	4.593(5)	4.011(9)
1523(100)	72.5(7)	73.80(4)	4.082(3)	4.555(3)	3.970(9)
1526(100)	70.9(6)	74.12(3)	4.098(2)	4.564(3)	3.963(7)
1529(100)	57.1(6)	78.09(6)	4.187(4)	4.615(4)	4.041(9)
1532(100)	64.9(6)	75.73(6)	4.121(4)	4.580(5)	4.013(9)
1533(100)	57.1(6)	78.08(5)	4.187(4)	4.615(4)	4.041(9)
1538(100)	66.0(6)	75.44(8)	4.112(5)	4.576(6)	4.010(9)
1542(100)	60.7(5)	76.54(6)	4.149(4)	4.597(4)	4.013(9)
1542(100)	66.3(6)	75.37(8)	4.110(6)	4.575(6)	4.008(9)
1543(100)	64.9(6)	75.74(8)	4.120(5)	4.578(6)	4.015(9)
1544(100)	64.5(6)	75.77(7)	4.122(5)	4.580(5)	4.013(9)
1582(100)	71.5(6)	74.11(2)	4.097(1)	4.564(1)	3.963(4)
1594(100)	60.6(5)	76.76(2)	4.151(2)	4.604(2)	4.016(5)
1615(100)	58.9(5)	77.11(4)	4.159(3)	4.609(3)	4.022(9)
1620(100)	58.1(6)	77.91(7)	4.184(5)	4.616(5)	4.035(9)
1629(100)	64.8(6)	75.86(6)	4.127(4)	4.581(5)	4.013(9)
1648(100)	61.4(6)	76.72(2)	4.149(2)	4.601(2)	4.019(5)

1648(100)	72.0(5)	74.05(4)	4.096(3)	4.564(3)	3.961(9)
1655(100)	61.5(6)	76.71(3)	4.147(2)	4.600(2)	4.021(6)
1656(100)	73.6(7)	73.77(3)	4.082(1)	4.555(2)	3.968(4)
1661(100)	70.0(6)	74.67(2)	4.105(1)	4.565(1)	3.985(3)
1673(100)	61.6(5)	76.56(4)	4.149(3)	4.597(3)	4.014(9)
1701(100)	61.5(5)	76.65(4)	4.151(3)	4.598(3)	4.016(8)
1704(100)	73.8(7)	73.82(2)	4.082(2)	4.555(2)	3.970(5)
1705(100)	56.0(5)	78.36(3)	4.201(2)	4.622(3)	4.036(7)
1728(100)	65.4(6)	75.80(6)	4.126(4)	4.581(5)	4.010(9)
1731(100)	65.5(6)	75.86(7)	4.126(5)	4.581(6)	4.014(9)
1734(100)	64.6(6)	76.10(5)	4.133(4)	4.591(4)	4.011(9)
1736(100)	65.6(6)	75.81(7)	4.125(5)	4.581(6)	4.011(9)
1740(100)	58.7(6)	77.31(4)	4.165(3)	4.609(3)	4.027(9)
1748(100)	65.5(6)	75.81(7)	4.127(5)	4.582(5)	4.009(9)
1785(100)	65.7(6)	75.83(6)	4.127(4)	4.581(5)	4.010(9)
1790(100)	65.8(6)	75.85(6)	4.127(4)	4.582(5)	4.011(9)
1792(100)	58.5(6)	77.27(5)	4.168(3)	4.612(4)	4.020(9)
1798(100)	70.6(6)	74.68(4)	4.105(1)	4.566(4)	3.985(4)
1813(100)	74.7(7)	73.74(2)	4.080(1)	4.555(1)	3.968(3)
1814(100)	62.1(6)	76.67(2)	4.153(1)	4.595(1)	4.017(4)
1816(100)	65.9(6)	75.85(6)	4.127(4)	4.581(5)	4.012(9)
1819(100)	66.0(6)	75.87(7)	4.127(5)	4.581(5)	4.013(9)
1820(100)	74.8(7)	73.78(1)	4.082(1)	4.554(1)	3.969(3)
1824(100)	62.8(6)	76.72(3)	4.147(2)	4.601(2)	4.021(6)
1832(100)	75.0(7)	73.77(3)	4.083(3)	4.554(3)	3.967(8)
1835(100)	63.0(6)	76.51(5)	4.147(4)	4.597(4)	4.013(9)
1840(100)	66.4(6)	75.82(7)	4.126(5)	4.581(5)	4.012(9)
1866(100)	62.8(6)	76.61(4)	4.150(3)	4.598(3)	4.015(8)
1873(100)	65.9(6)	75.87(7)	4.128(5)	4.583(6)	4.011(9)
1897(100)	71.1(6)	74.54(4)	4.105(1)	4.567(1)	3.976(2)
1937(100)	63.4(6)	76.75(3)	4.147(2)	4.601(3)	4.023(7)
1956(100)	62.8(6)	76.84(4)	4.152(3)	4.605(3)	4.019(8)
1962(100)	67.0(6)	75.74(6)	4.128(4)	4.582(4)	4.004(9)
1992(100)	67.5(6)	75.83(6)	4.126(4)	4.582(5)	4.011(9)
1999(100)	71.8(6)	74.47(2)	4.105(2)	4.567(2)	3.972(5)
2015(150)	66.9(7)	75.87(6)	4.128(4)	4.583(5)	4.010(9)
2029(150)	57.8(6)	78.03(2)	4.192(1)	4.623(1)	4.026(1)
2037(150)	67.3(7)	75.86(6)	4.128(4)	4.582(5)	4.010(9)
2054(150)	60.0(7)	77.20(2)	4.170(1)	4.611(2)	4.015(4)
2061(150)	67.8(7)	75.78(5)	4.128(4)	4.583(4)	4.006(9)
2069(150)	58.4(6)	77.96(2)	4.190(2)	4.624(2)	4.024(5)
2080(150)	67.7(7)	75.79(5)	4.127(4)	4.582(4)	4.008(9)
2103(150)	72.7(8)	74.52(4)	4.106(1)	4.567(1)	3.974(2)
2139(150)	64.2(7)	76.64(3)	4.151(2)	4.598(2)	4.015(5)

2160(150)	61.1(7)	77.18(1)	4.166(1)	4.609(1)	4.019(2)
-----------	---------	----------	----------	----------	----------

^a Numbers in parentheses are uncertainties on the last digits.