

Supplementary Material to the article

"Reevaluating CaCO_3 behavior at high pressure: formation of Ca_2CO_4 under reduced conditions"

Table S1. The unit cell parameters of Ca_2CO_4 -*Pnma* obtained in M1127 experiment at various pressures and temperatures.

$a(\text{Au}), \text{\AA}$	$V(\text{Au}), \text{\AA}^3$	P, GPa	T, K	$a (\text{\AA})$	$b (\text{\AA})$	$c (\text{\AA})$	Volume (\AA^3)
3.9575(2)	61.983(8)	27.409	1673	6.2480(5)	4.9084(7)	8.3950(29)	257.455(68)
3.9595(2)	62.075(8)	27.592	1773	6.2610(5)	4.8878(7)	8.4608(30)	258.922(70)
3.9555(2)	61.885(8)	26.781	1473	6.2531(5)	4.8752(7)	8.4480(14)	257.536(36)
9.9508(2)	61.668(8)	26.904	1373	6.2473(5)	4.8725(7)	8.4469(14)	257.121(36)
3.9479(2)	61.531(8)	26.674	1273	6.2447(5)	4.8685(7)	8.4399(14)	256.592(36)
3.9428(2)	61.293(8)	26.235	1073	6.2380(5)	4.8647(7)	8.4394(14)	256.101(36)
3.9406(2)	61.189(8)	25.851	873	6.2328(5)	4.8497(7)	8.4383(14)	255.063(36)
3.9381(2)	61.073(8)	25.446	673	6.2277(5)	4.8488(7)	8.4366(14)	254.760(36)
3.9353(2)	60.944(8)	24.987	473	6.2242(5)	4.8394(7)	8.4228(14)	253.708(35)
3.9326(2)	60.817(8)	24.633	300	6.2217(5)	4.8374(7)	8.4139(13)	253.232(35)
3.9504(2)	61.650(8)	20.879	300	6.2491(5)	4.8645(7)	8.4639(11)	257.293(38)
3.9624(2)	62.211(8)	22.968	1073	6.2642(5)	4.8917(7)	8.4797(11)	259.841(38)
3.9664(2)	62.399(8)	23.596	1273	6.2788(5)	4.898(7)	8.4795(11)	260.787(39)
3.9668(2)	62.419(8)	23.809	1373	6.2800(5)	4.8982(7)	8.4844(11)	260.987(39)
3.9678(2)	62.468(8)	24.017	1473	6.2782(5)	4.9029(7)	8.4945(11)	261.470(39)
3.9750(2)	62.808(9)	24.171	1573	6.2880(5)	4.9117(7)	8.4946(11)	262.355(39)
3.9768(2)	62.894(9)	24.332	1673	6.2845(5)	4.9110(9)	8.5145(11)	262.781(41)
3.9621(2)	62.199(8)	23.931	1773	6.2990(5)	4.9115(7)	8.5023(11)	263.040(33)
3.9670(2)	62.429(8)	23.236	1273	6.2758(5)	4.8957(7)	8.4950(11)	261.003(39)
3.9593(2)	62.065(8)	22.164	873	6.2634(5)	4.8796(7)	8.4781(11)	259.112(38)
3.9536(2)	61.796(8)	21.901	673	6.2514(5)	4.8767(7)	8.4767(11)	258.421(38)
3.9505(2)	61.654(8)	21.366	473	6.2483(4)	4.8738(7)	8.4645(11)	257.768(38)
3.9450(2)	61.395(8)	21.101	300	6.2418(4)	4.8703(7)	8.4630(11)	257.271(38)
3.9653(2)	62.349(8)	17.717	300	6.2663(4)	4.8967(6)	8.5042(11)	260.941(34)
3.9811(2)	63.097(9)	20.684	1273	6.2976(4)	4.9238(6)	8.5423(11)	264.880(35)
3.9877(2)	63.413(9)	20.446	1473	6.3148(4)	4.9357(6)	8.5461(11)	266.364(35)

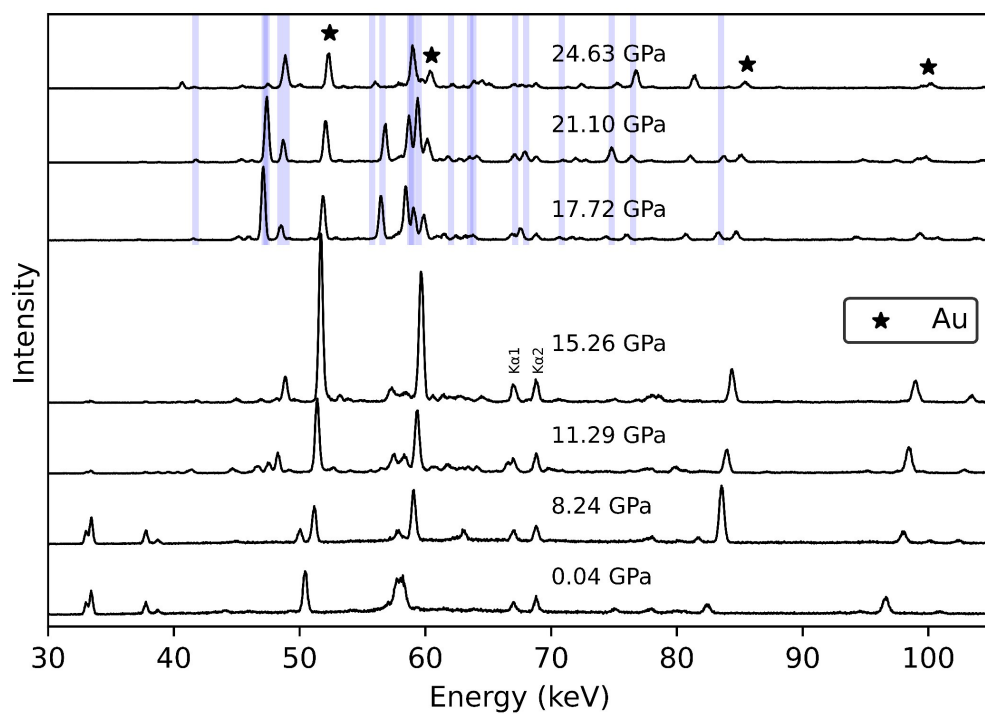


Figure S1. The diffraction patterns obtained at various pressures; blue bands indicate the peaks positions of Ca_2CO_4 - $Pnma$.