

Article

High-Pressure Phase Diagrams of Na_2CO_3 and K_2CO_3

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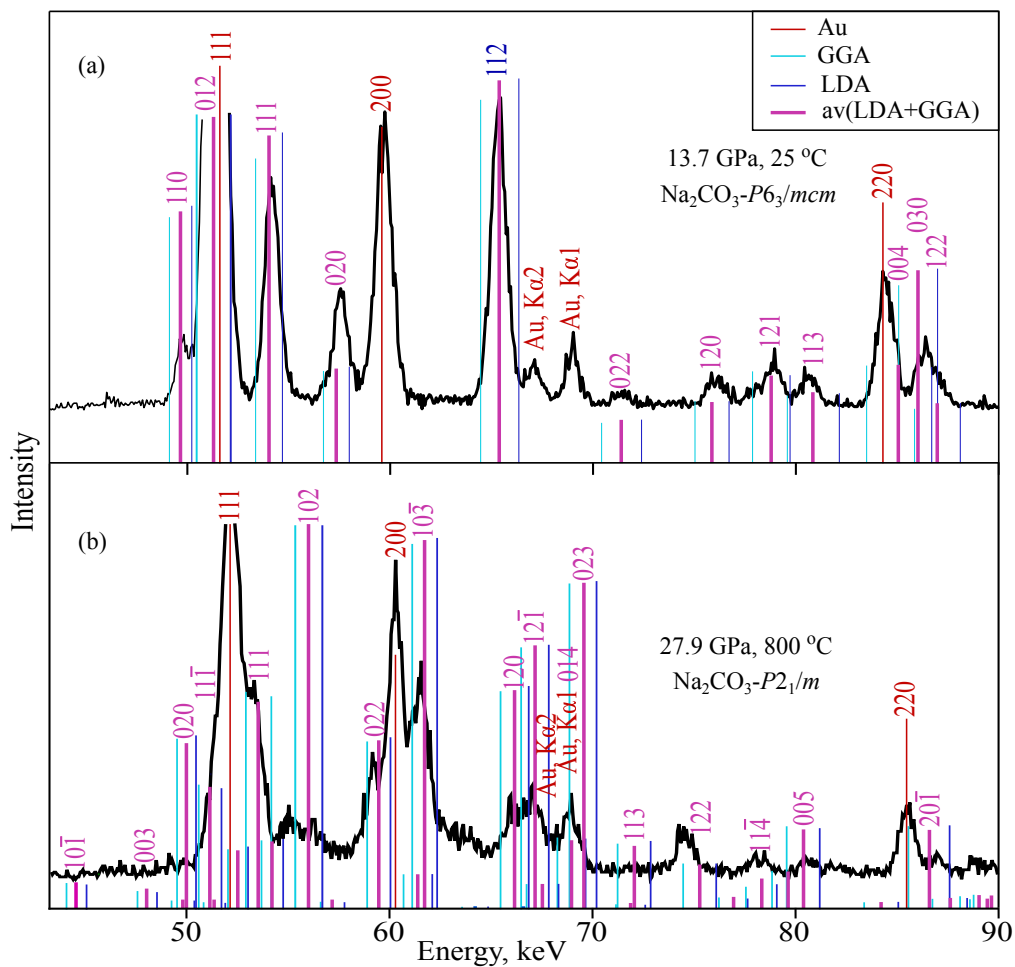


Figure S1. Experimental diffraction patterns at 13.7 GPa (a) and at 27.9 GPa (b) with theoretical peaks of $\text{Na}_2\text{CO}_3\text{-}P6_3/mcm$ (a) and $\text{Na}_2\text{CO}_3\text{-}P2_1/m$ (b) structures. Peaks of the structure optimised with LDA are shown with thin blue lines, with GGA – with turquoise thin lines, and of the averaged structure – with thick violet lines

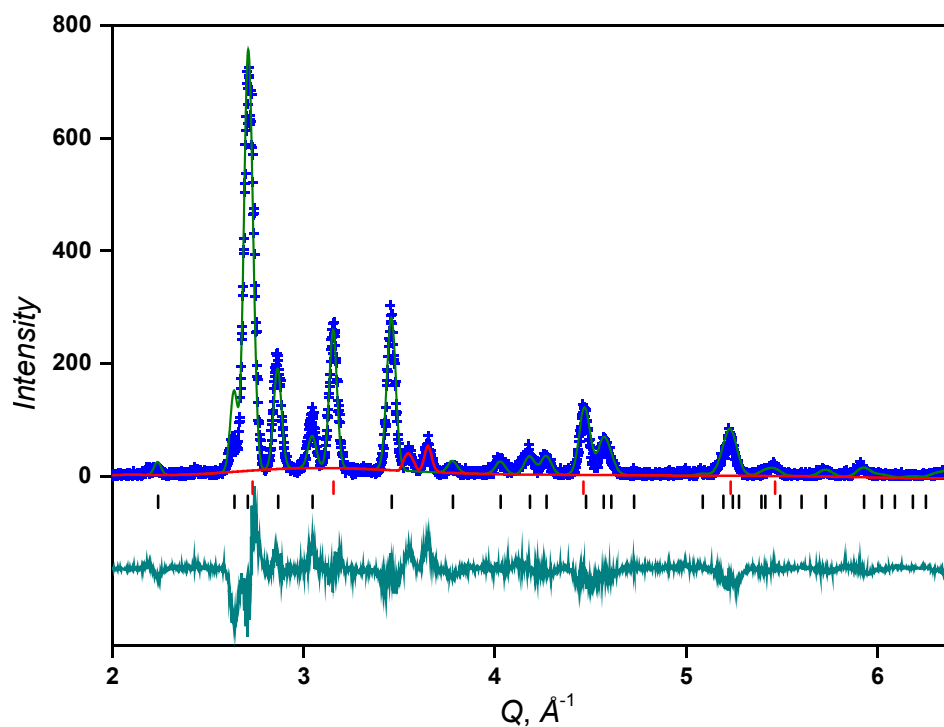


Figure S2. Rietveld refinement of $\text{Na}_2\text{CO}_3\text{-}P6_3/mcm$ structure with MA diffraction pattern recorded at 13.7 GPa and 27 °C, R-factor=27%

Table S1. Unit cell parameters of $\gamma\text{-Na}_2\text{CO}_3$ from DAC-APS experiments

Pressure (GPa)	Temperature (°C)	Unit cell parameters (Å, deg.)				Volume (Å ³)
		<i>a</i>	<i>b</i>	<i>c</i>	<i>β</i>	
γ-Na ₂ CO ₃ (DAC-APS)						
2.8	25	8.89(2)	5.32(5)	5.94(4)	104.84(8)	271.6(1)
5.9	25	8.67(2)	5.16(5)	5.78(4)	103.21(8)	252.1(1)
7.6	25	8.62(2)	5.13(5)	5.72(4)	103.60(8)	245.7(1)
9.5	25	8.51(2)	5.20(5)	5.72(4)	105.67(8)	243.5(1)
11.8	25	8.47(2)	5.155(4)	5.67(4)	105.65(8)	238.2(1)
12.5	25	8.45(2)	5.15(5)	5.66(4)	105.73(8)	237.1(1)
14.1	25	8.43(2)	5.16(5)	5.62(4)	105.52(8)	235.2(1)
16.2	25	8.45(2)	5.15(5)	5.56(4)	104.76(8)	233.8(1)
18.0	25	8.44(2)	5.12(5)	5.59(4)	105.90(8)	232.5(1)
24.0	25	8.36(2)	5.06(5)	5.58(4)	106.33(8)	226.2(1)

Table S2. Structural data of $\text{K}_2\text{CO}_3\text{-}C2/m$ used for indexing of experimental diffraction pattern (according to DFT calculations, without refinement)

Pr.,Temp. (GPa, °C)	Space group	Lattice parameters			Species	Atomic coordinates		
		Å, deg.				<i>x</i>	<i>y</i>	<i>z</i>
K ₂ CO ₃ -P2 ₁ /m								
20.1, 25	P2 ₁ /m	<i>a</i> = 2.99	<i>b</i> = 5.18	<i>c</i> = 6.55	K1	0.01	0.75	0.53
		<i>α</i> =90	<i>β</i> = 97.47	<i>γ</i> = 90	K2	0.09	0.75	0.88
					C1	0.49	0.25	0.76
					O1	0.56	0.04	0.69
					O2	0.56	0.46	0.69
					O3	0.34	0.25	0.89

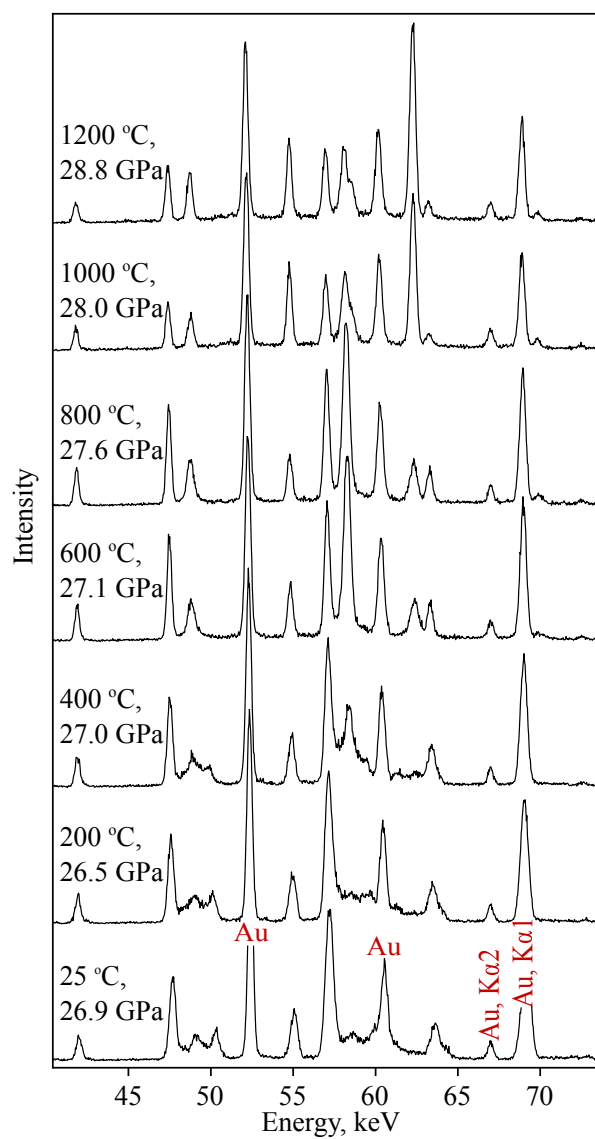


Figure S3. Changes of diffraction pattern on heating at pressures 26.9–28.8 GPa according to MA setting

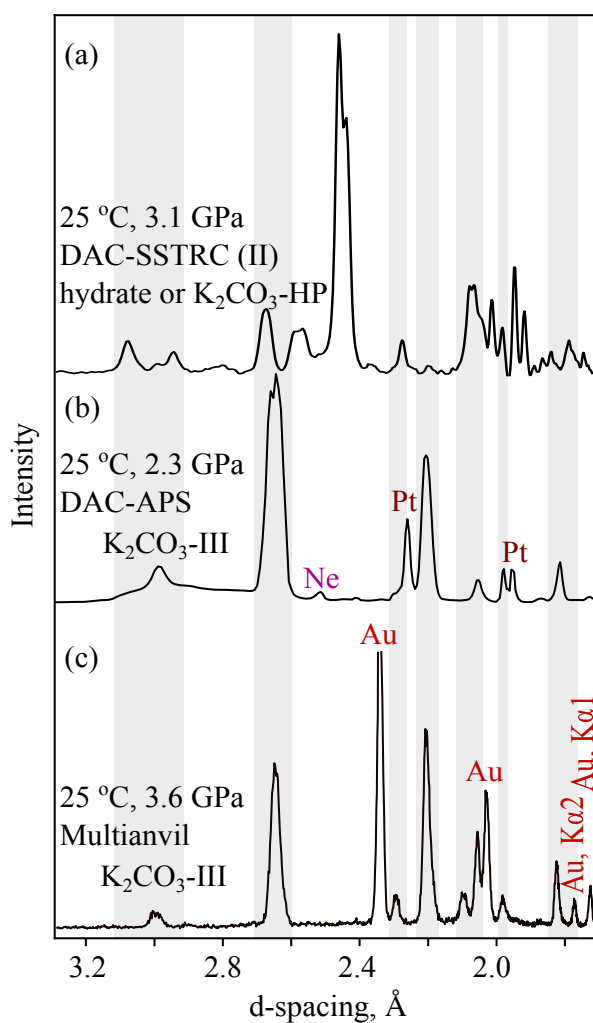


Figure S4. Diffraction patterns in DAC-SSTRC (a), DAC-APS (b), and multianvil (c) settings at 2.3-3.6 GPa. Grey bands are shown for the convenience of visual comparison

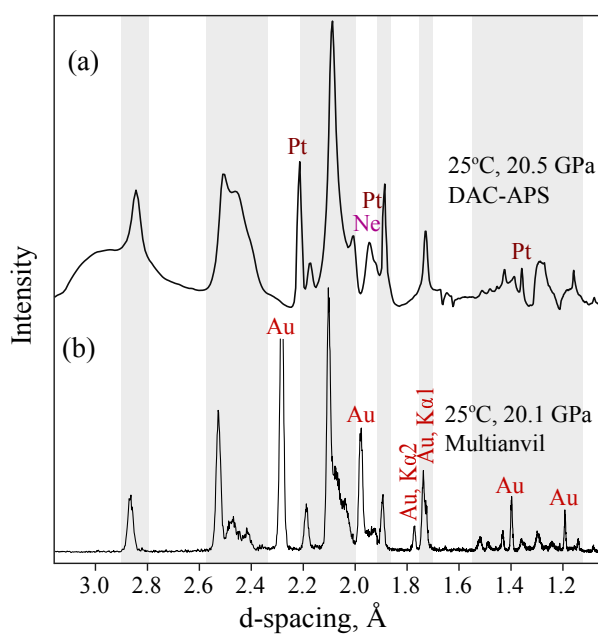


Figure S5. Diffraction patterns of K_2CO_3 -IV recorded in DAC-APS (a) and multianvil (b) settings

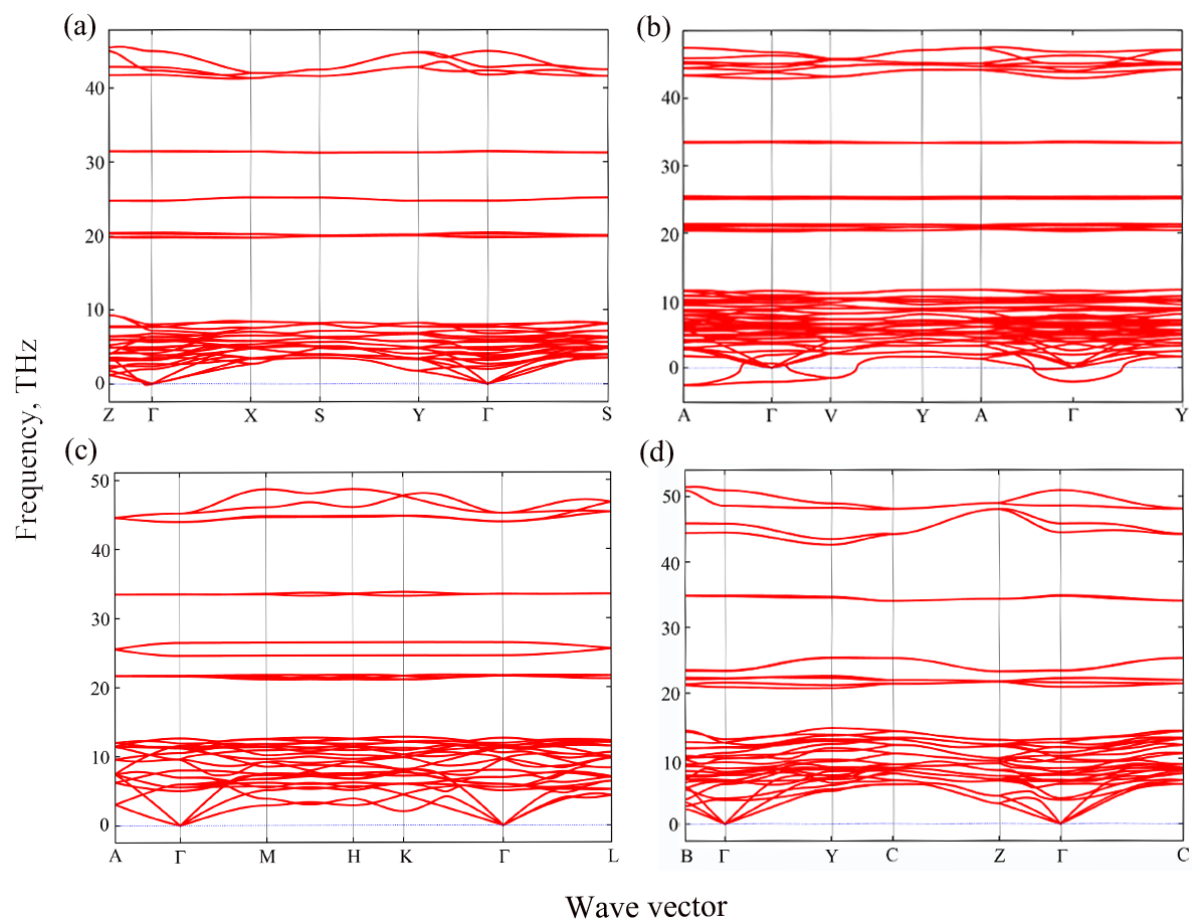


Figure S6. Phonon dispersion curves of Na_2CO_3 phases, $Pmmn$ at 0 GPa (a), γ at 12 GPa (b), and $P6_3/mcm$ at 24 GPa (c) and $P2_1/m$ at 36 GPa (d)

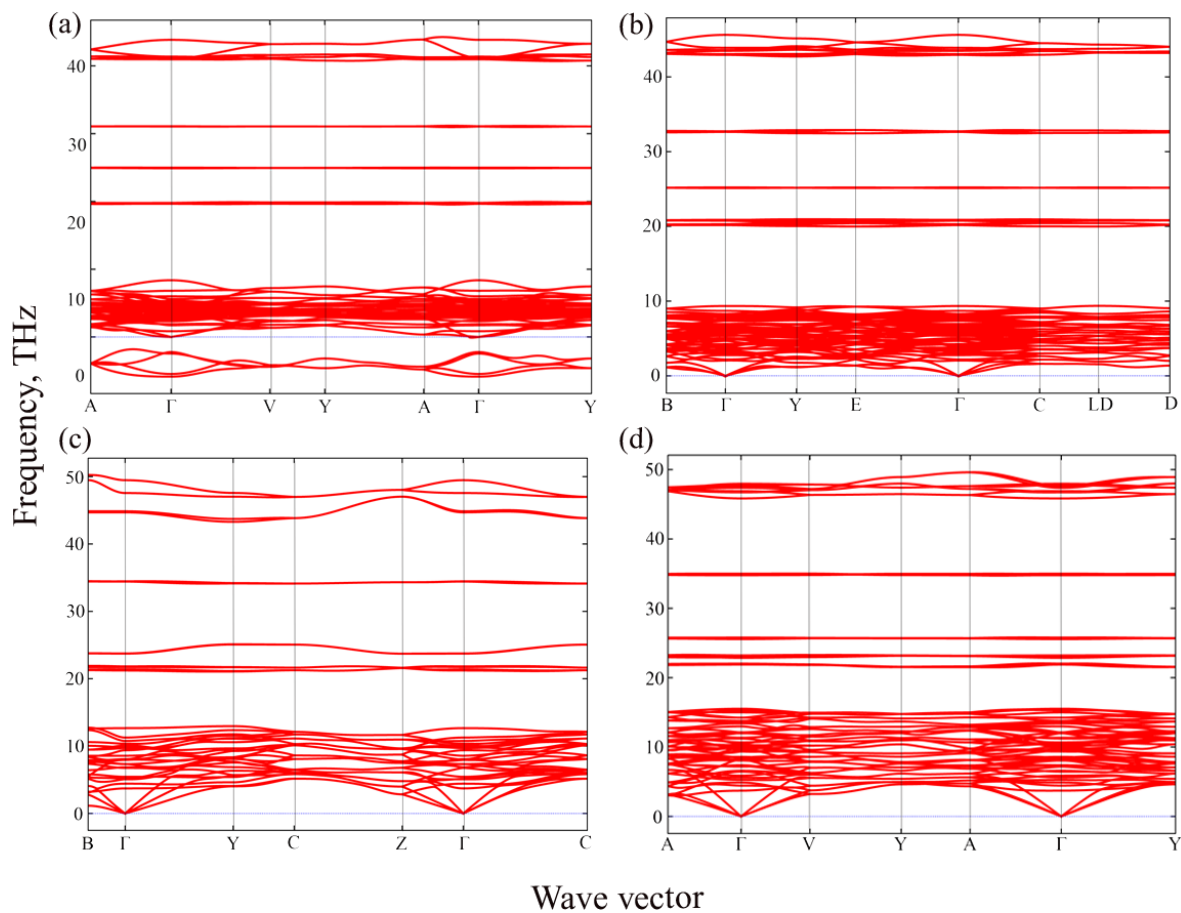


Figure S7. Phonon dispersion curves of K_2CO_3 phases, β at 0 GPa (a), γ at 1 GPa (b), $P2_1/m$ at 36 GPa (c) and $C2/c$ at 60 GPa (d)

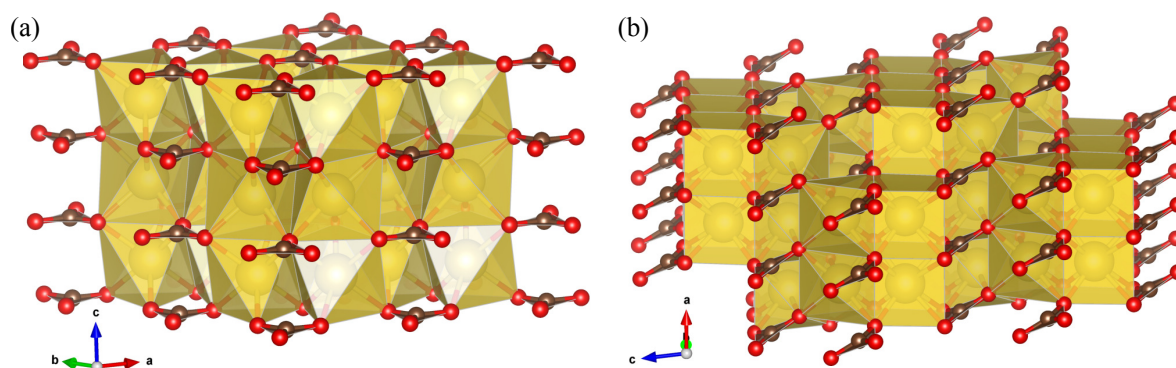


Figure S8. Na-O polyhedrons in $P6_3/mcm$ (a) and $P2_1/m$ (b) crystal structures of Na_2CO_3



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