

Supplemental Information

New pressure-induced phase transition to Co₂Si-type Fe₂P

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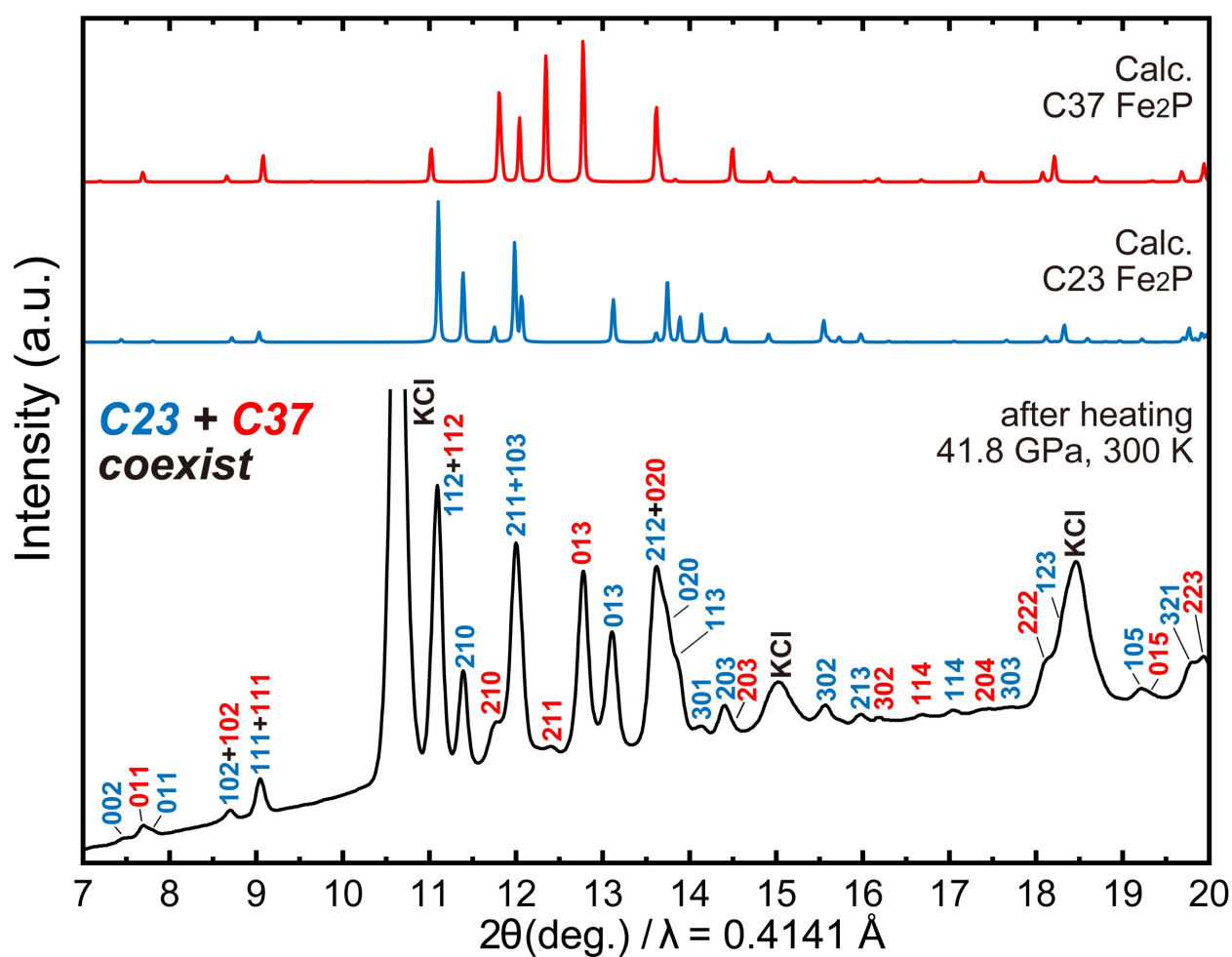


FIGURE S1. XRD pattern of Fe₂P at 41.8 GPa and 300 K in run #3. C23 and C37 phases coexisted upon and after heating at ~42 GPa. Mirror indexes in blue and red are for peaks from C23 and C37, respectively. For comparison, powder diffraction patterns for C23 and C37 are calculated based on the measured lattice parameters given in [TABLE S2](#).

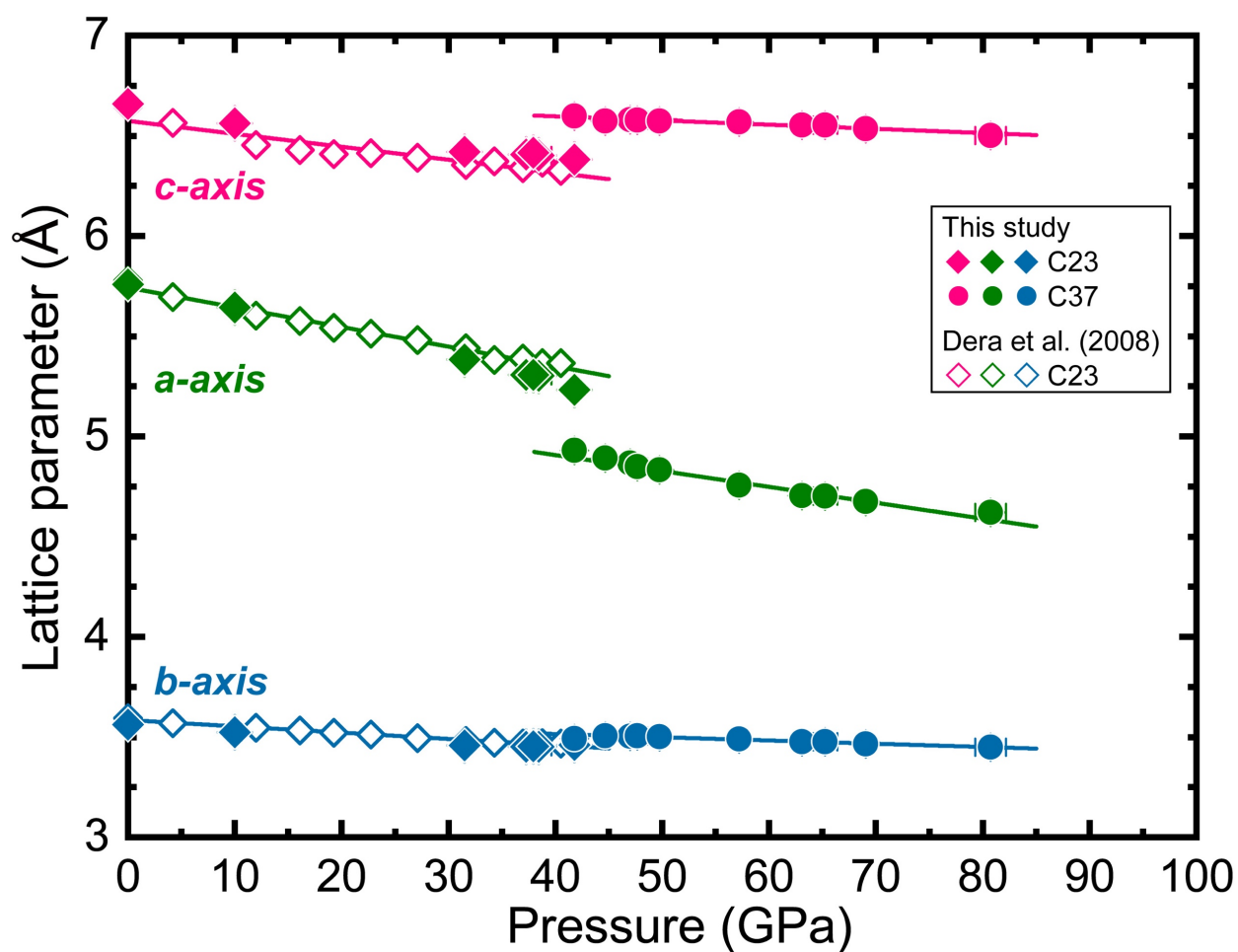


FIGURE S2. Lattice parameters of C23 (triangles) and C37 Fe₂P (circles) at 300 K. Filled and open symbols are from this study and Dera et al. (2008), respectively. Lines are for eyes.

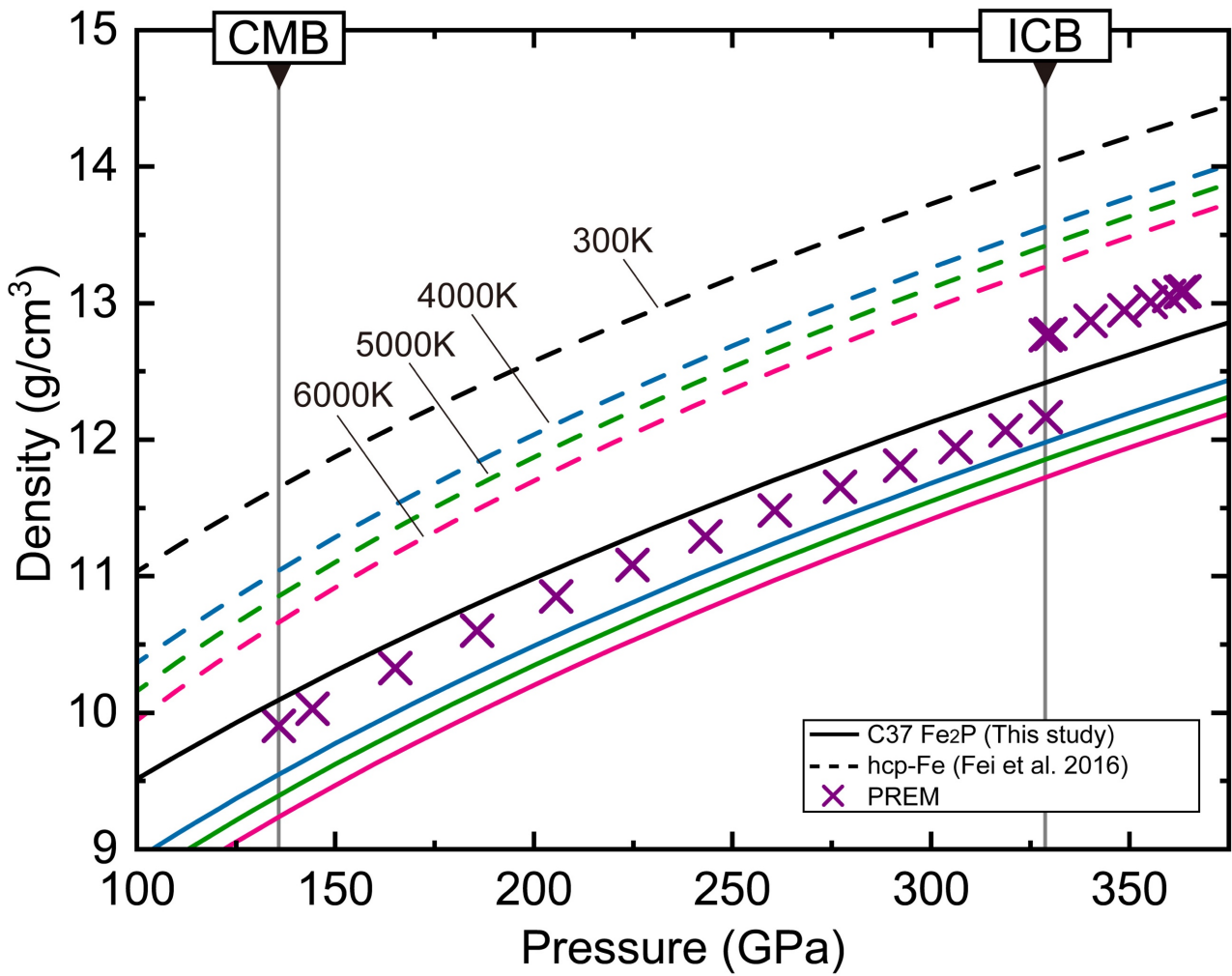


FIGURE S3. Densities of C37 Fe₂P (solid lines) and hcp Fe (broken lines, Fei et al. 2016) under core pressures at 300 K (black), 4000 K (blue), 5000 K (green), and 6000 K (magenta). Seismologically-deduced PREM density profile is given by purple crosses (Dziewonski and Anderson 1981).

TABLE S1. High P - T run conditions and stable phases

Run #	P (GPa)	T (K) ^a	Stable phase
1	35.4(8)	1650	C23
	36.4(11)	1310	C23
	39.3(15)	1340	C23
	51.5(9)	1650	C37
	52.1(12)	1760	C37
	60.9(9)	1830	C37
	67.6(13)	2330	C37
	73.5(28)	2130	C37
2	69.4(9)	2100	C37
3	39.6(17)	1360	C23
	42.4(9)	1250	C23+C37
	43.5(7)	1380	C23+C37
	48.2(17)	1400	C37
	48.8(26)	1490	C37
	38.5(11)	1350	C23
	12.1(7)	1300	C23
4	71.7(47)	1780	C37
	83.3(11)	1680	C37

^a Temperature uncertainty is $\pm 10\%$.

TABLE S2. Volumes of C23 and C37 Fe₂P at 300 K

Run #	<i>P</i> (GPa)	<i>T</i> (K)	<i>V</i> (Å ³)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	Phase
1	31.5(1)	300	119.5(2)	5.383(3)	3.459(2)	6.421(3)	C23
	38.4(12)	300	117.2(2)	5.303(3)	3.451(2)	6.403(3)	C23
	47.0(9)	300	112.2(2)	4.867(2)	3.504(2)	6.580(2)	C37
	49.8(6)	300	111.2(2)	4.834(2)	3.501(1)	6.574(2)	C37
	57.2(0)	300	109.1(1)	4.757(1)	3.490(1)	6.570(1)	C37
	63.1(5)	300	107.1(1)	4.705(2)	3.475(1)	6.553(2)	C37
	69.0(6)	300	105.9(1)	4.674(2)	3.466(1)	6.536(2)	C37
3	37.3(1)	300	117.3(2)	5.307(3)	3.451(2)	6.406(3)	C23
	41.8(2)	300	115.6(3)	5.233(4)	3.461(3)	6.382(4)	C23 ^a
		300	113.6(4)	4.929(6)	3.493(4)	6.599(6)	C37 ^a
	44.7(9)	300	112.7(2)	4.891(2)	3.506(2)	6.573(2)	C37
	47.7(9)	300	111.8(2)	4.848(2)	3.505(2)	6.578(3)	C37
	37.9(8)	300	117.6(2)	5.306(2)	3.454(1)	6.416(2)	C23 ^b
	10.0(2)	300	130.4(4)	5.642(4)	3.523(5)	6.561(4)	C23 ^b
	0.0(0)	300	136.6(3)	5.758(4)	3.562(2)	6.659(3)	C23 ^b
4	65.3(11)	300	107.1(2)	4.702(2)	3.477(2)	6.553(2)	C37
	80.7(14)	300	103.6(2)	4.62(2)	3.450(2)	6.501(2)	C37

^a C23 and C37 phases coexisted.^b Data were collected upon decompression.