

Supporting Information

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Table S1. Comparison of observed powder X-ray diffraction (XRD) peaks collected from Ca-III at 37 GPa and 300 K with those calculated using a simple-cubic (sc) unit cell, $a = 2.6750(5)$ Å, and a rhombohedral (rh) ($R\bar{3}m$) unit cell, $a = 2.6750(5)$ Å, $\alpha = 89.90(1)^\circ$

sc				$R\bar{3}m$		
<i>hkl</i>	d_{obs} (Å)	d_{calc} (Å)	Δd (Å)	<i>hkl</i>	d_{calc} (Å)	
100	2.6744	2.6750	-0.0006	100	2.6750	
110	1.8922	1.8915	0.0007	110	1.8932	
				110	1.8899	
111	1.5443	1.5444	-0.0001	111	1.5471	
				111	1.5435	
200	1.3378	1.3375	0.0003	200	1.3375	
210	1.1963	1.1965	-0.0002	210	1.1971	
				210	1.1955	
211	1.0917	1.0921	-0.0004	211	1.0937	
				211	1.0917	
				211	1.0911	
220	0.9455	0.9458	-0.0003	220	0.9466	
				220	0.9449	
221	0.8918	0.8917	0.0001	221	0.8931	
				221	0.8917	
				221	0.8910	
300	0.8918	0.8917	0.0001	300	0.8917	
310	0.8459	0.8459	0.0000	310	0.8464	
				310	0.8455	
311	0.8063	0.8065	-0.0002	311	0.8074	
				311	0.8064	
				311	0.8059	
222	0.7721	0.7722	-0.0001	222	0.7736	
				222	0.7718	
320	0.7420	0.7419	0.0001	320	0.7425	
				320	0.7413	
321	0.7150	0.7149	0.0001	321	0.7159	
				321	0.7150	
				321	0.7145	
				321	0.7143	

Table S2. Comparison of observed single crystal XRD spot d spacings collected from Ca-III at 42 GPa and 300 K with those calculated using a rh ($R\bar{3}m$) unit cell, $a = 2.6684(5)$ Å, $\alpha = 89.90(1)^\circ$, and a sc unit cell, $a = 2.6684(5)$ Å

$R\bar{3}m$				sc	
<i>hkl</i>	d_{obs} (Å)	d_{calc} (Å)	Δd (Å)	d_{calc} (Å)	Δd
100	2.6684	2.6675	0.0009	2.6675	0.0009
110	1.8873	1.8878	-0.0005	1.8862	0.0011
110	1.8842	1.8846	-0.0004	1.8862	-0.0020
111	1.5423	1.5427	-0.0004	1.5401	0.0022
111	1.5387	1.5392	-0.0005	1.5401	-0.0014
200	1.3339	1.3338	0.0001	1.3338	0.0001
210	1.1936	1.1938	-0.0002	1.1929	0.0007
210	1.1922	1.1921	0.0001	1.1929	-0.0007
221	0.8913	0.8905	0.0008	0.8892	0.0021
221	0.8898	0.8892	0.0006	0.8892	0.0006
221	0.8976	0.8885	-0.0009	0.8892	-0.0016
300	0.8885	0.8892	-0.0007	0.8892	-0.0007

