Supplement Information for

Exploring the superconductivity of $CaSrB_5$: High-Pressure Stability and Electron-Phonon Interactions

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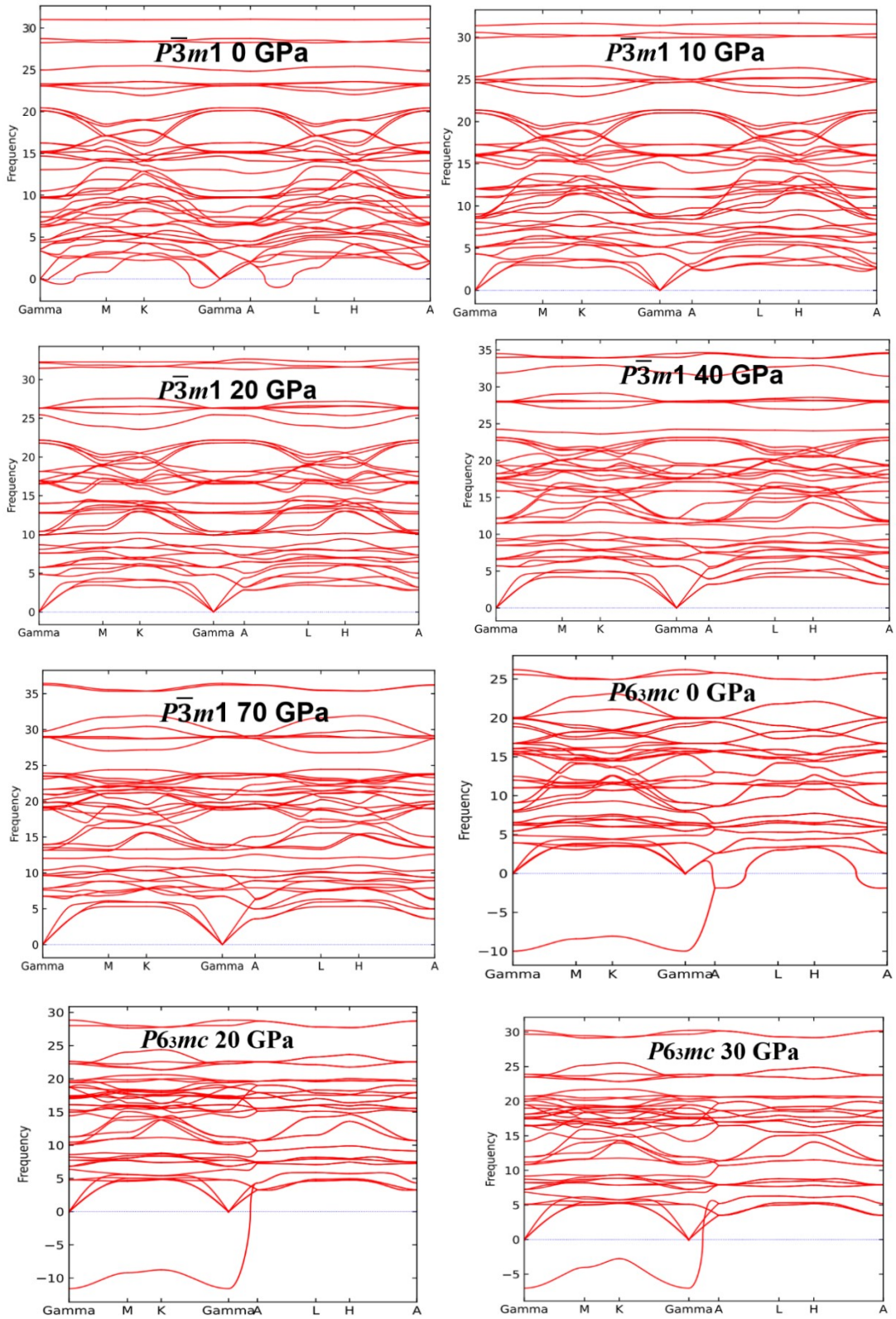
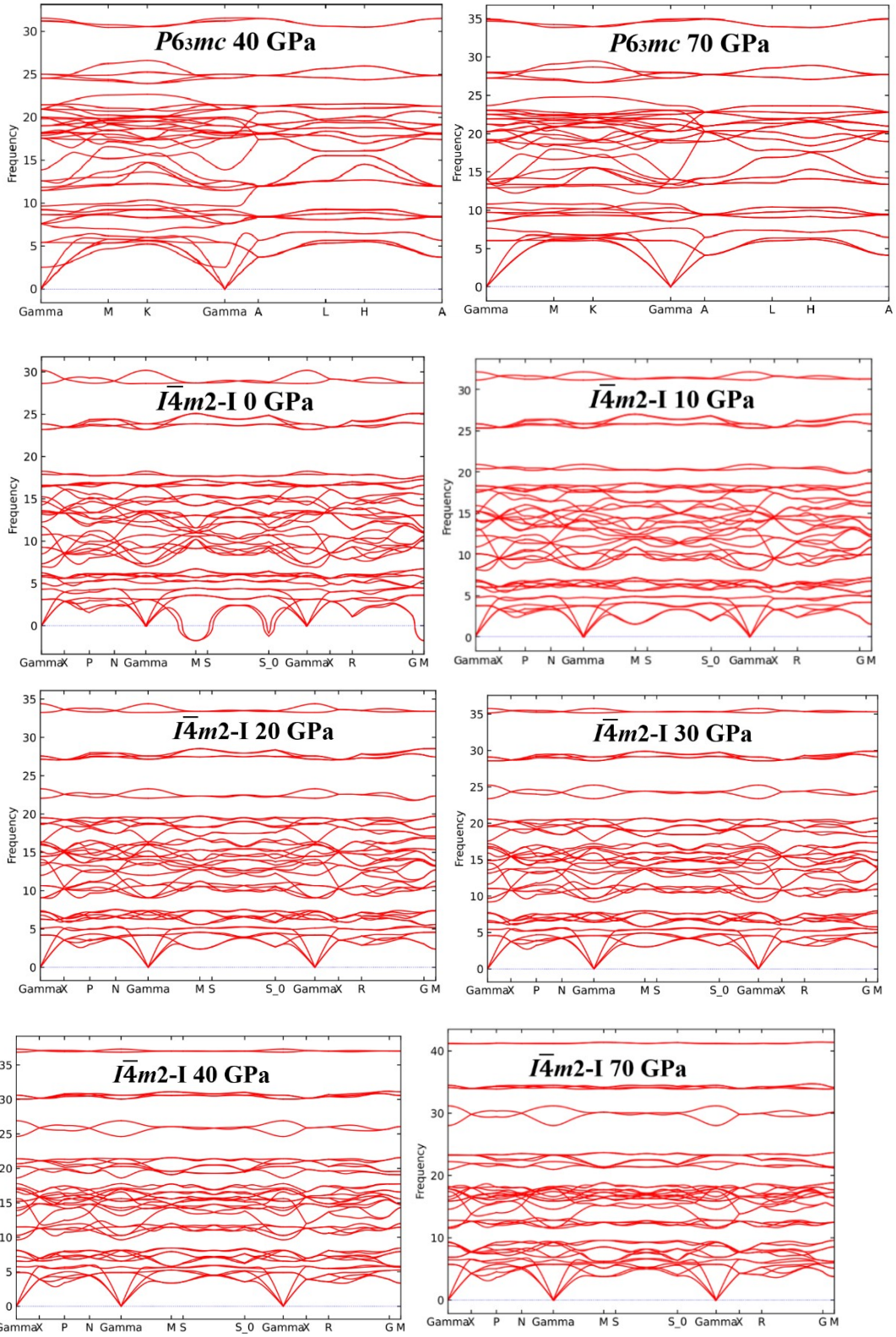

$P\bar{3}m1$ 0 GPa
$P\bar{3}m1$ 10 GPa
$P\bar{3}m1$ 20 GPa
$P\bar{3}m1$ 40 GPa
$P\bar{3}m1$ 70 GPa
$P6_3mc$ 0 GPa
$P6_3mc$ 20 GPa
$P6_3mc$ 30 GPa
Frequency
Gamma M K Gamma A L H A


P6₃mc 40 GPa
P6₃mc 70 GPa
I4̄m2-I 0 GPa
I4̄m2-I 10 GPa
I4̄m2-I 20 GPa
I4̄m2-I 30 GPa
I4̄m2-I 40 GPa
I4̄m2-I 70 GPa
Frequency
Gamma M K Gamma A L H A
GammaX P N Gamma M S S_0 GammaX R G M

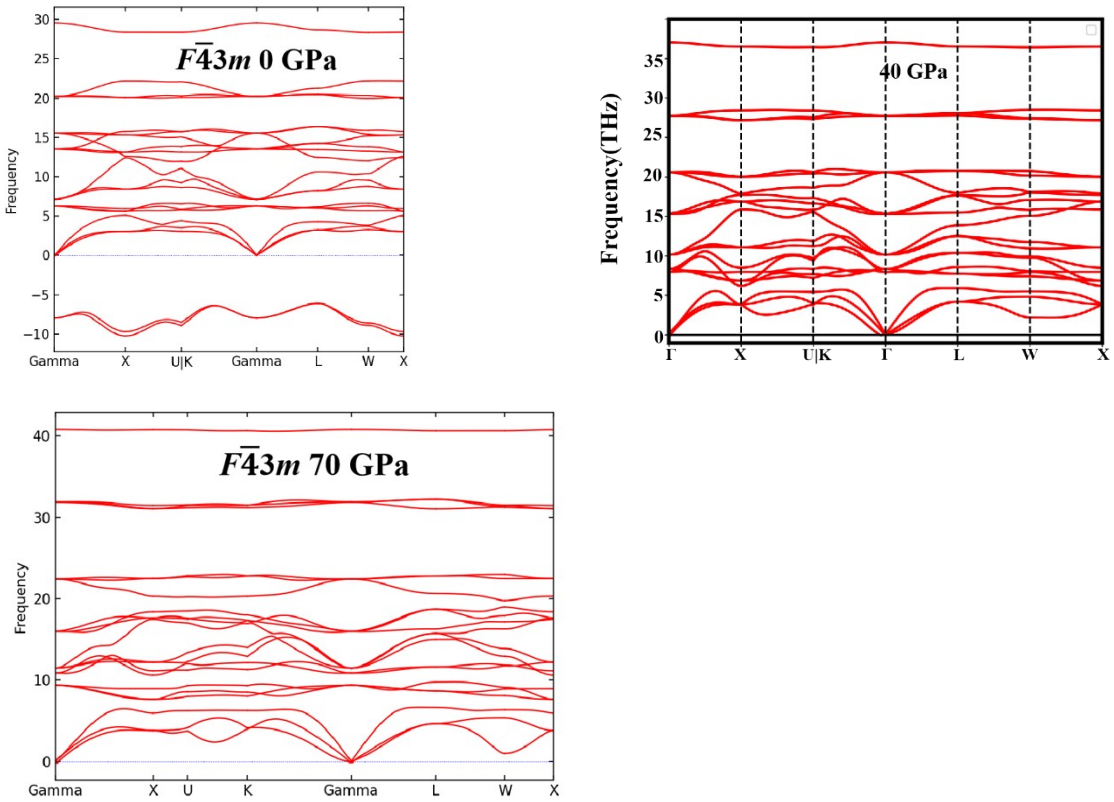
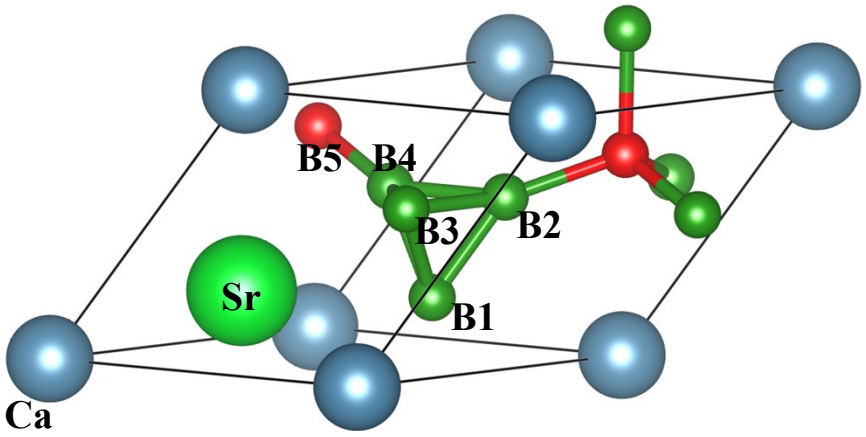


FIG. S1 The phonon spectrum of $F\bar{4}3m$, $I\bar{4}m2$-I, $P6_3mc$ and $P\bar{3}m1$ phase at various pressure by phonopy codes [1].

Table S1. The bond lengths of $F\bar{4}3m$ phase, $I\bar{4}m2$ phase by moving atoms and USPEX.



	$F\bar{4}3m$ $CaSrB_5$	$I\bar{4}m2$-II	$I\bar{4}m2$-III	$I\bar{4}m2$-I

d(Ca-Ca)	4.562	4.562	4.562	4.547
d(Ca-Sr)	2.794	2.784	2.794	2.797
d(Sr-Sr)	4.562	4.562	4.562	4.547
d(B1-B2) = d(B3-B4)	1.706	1.695	1.730	1.795
d(B1-B3) = d(B2-B3) = d(B1-B4) = d(B2-B4)	1.706	1.712	1.695	1.668
d(B4-B5)	1.749	1.749	1.749	1.752
d(Ca-B5)	2.794	2.794	2.794	3.260
d(Sr-B5)	3.226	3.226	3.226	2.797

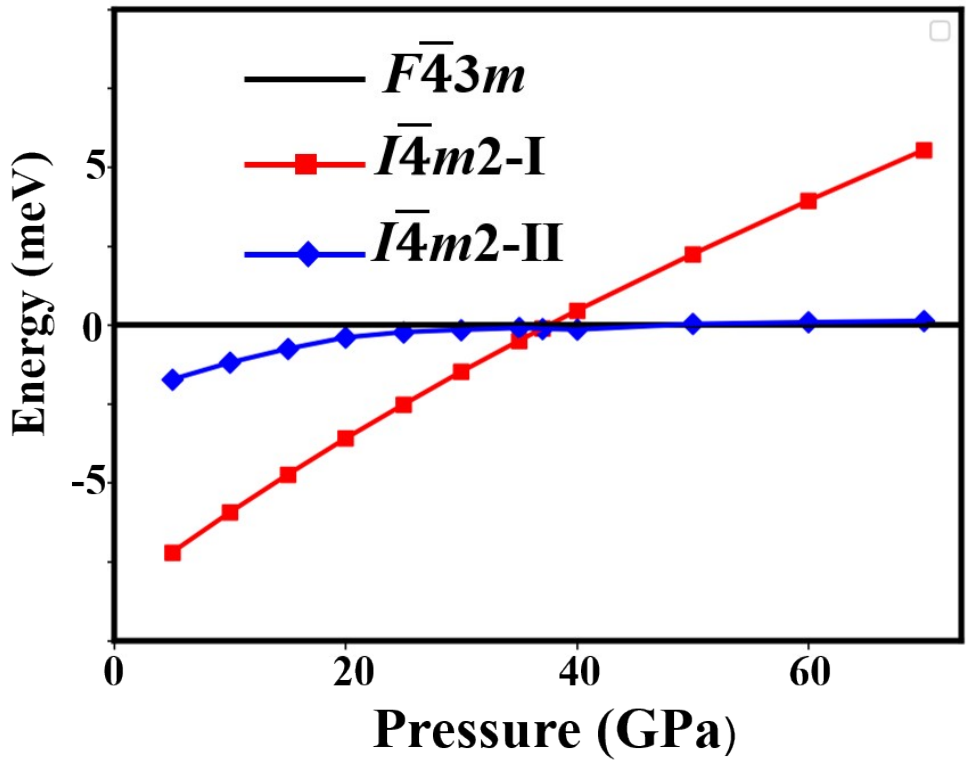


FIG. S2 The enthalpy differences between the $F\bar{4}3m$, $I\bar{4}m2$-I and $I\bar{4}m2$-II phases at range of 0 – 70 GPa.

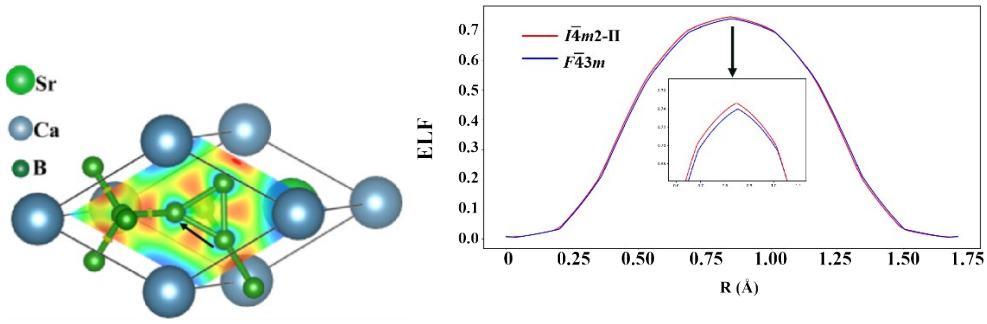


FIG. S3 The ELF values across the B-B bond (along the black line) of $F\bar{4}3m$ and $I\bar{4}m2$-II phases.

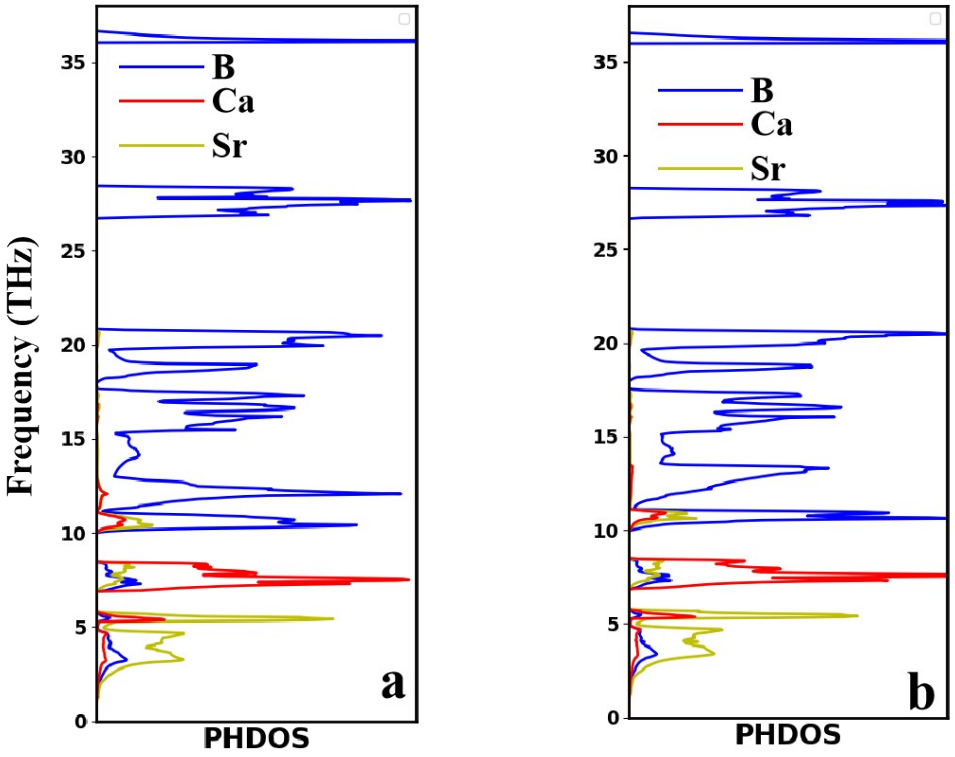


FIG. S4 the phdos of $CaSrB_5$ under both (a) harmonic and (b) anharmonic approximations

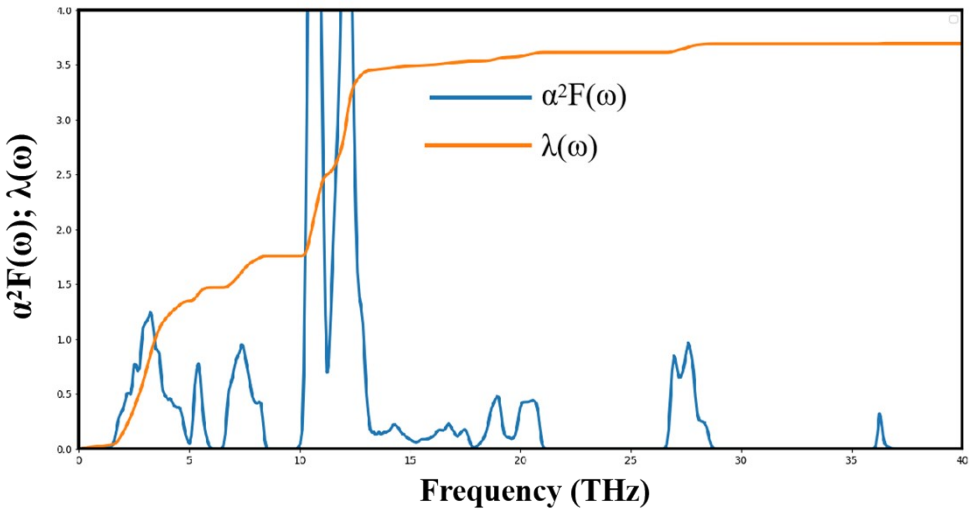


FIG. S5. Eliashberg spectral function $\alpha^2F(\omega)$, and accumulated $\lambda(\omega)$ for $F\bar{4}3m$ phase by EPW codes[2]

Table S2. The Predicted structural parameters of $CaSrB_5$ compounds at 40 GPa

structure	Lattice paremeters	atoms	(X, Y, Z)
$F\bar{4}3m$	a=b=c=6.365Å	Ca(4a)	(0.500, 0.000, 0.500)
	α=β=γ=90°	Sr(4c)	(0.750, 0.750, 0.250)
		B(16e)	(0.406, 0.906, 0.094)
		B(4d)	(0.750, 0.750, 0.750)
$P\bar{3}m1$	a=b=4.370 Å	Ca(2d)	(0.333,0.667,0.433)
	c=7.743 Å	Sr(2d)	(0.333,0.667,0.065)
	α=β=90°	B(2c)	(0.000,0.000,0.831)
	γ=120°	B(2c)	(0.000,0.000,0.391)
		B(6i)	(0.204,0.796,0.736)
$I\bar{4}m2$-I	a=b=4.552 Å	Ca(2c)	(0.000, 0.500,0.250)
	c=6.242 Å	Sr(2a)	(0.500, 0.500, 0.500)
	α=β=γ=90°	B(8i)	(0.695,0.500,0.914)
		B(2d)	(0.500,0.000.0.250)
	a=b=4.369 Å	Ca(2b)	(0.667,0.333,0.097)
	c=7.614 Å	Sr(2b)	(0.333,0.667,0.969)
$P6_3mc$	α=β=90°	B(2a)	(0.000,0.000,0.161)
	γ=120°	B(2a)	(0.000,0.000,0.404)
		B(6c)	(0.202,0.798,0.282)

REFERENCES

[1] A. Togo, I. Tanaka, Scr. Mater.2015, **108**, 1-5.
[2] S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, *Comp. Phys. Commun.* 2016, **209**, 116.