

Supplementary Information

Octahedron rotation evolution in 2D perovskites and its impact on optoelectronic properties: the case of Ba-Zr-S chalcogenides

Chen Ming^a, Ke Yang^{b, c}, Hao Zeng^d, Shengbai Zhang^b, Yi-Yang Sun^{a,*}

^a *State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, 201899, China*

^b *Department of Physics, Applied Physics & Astronomy, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA*

^c *School of Physics and Electronics, Hunan University, Changsha, 410082, China*

^d *Department of Physics, University at Buffalo, The State University of New York, Buffalo, NY, 14260, USA*

* Corresponding Author.

Email address: yysun@mail.sic.ac.cn (Y.-Y. Sun)

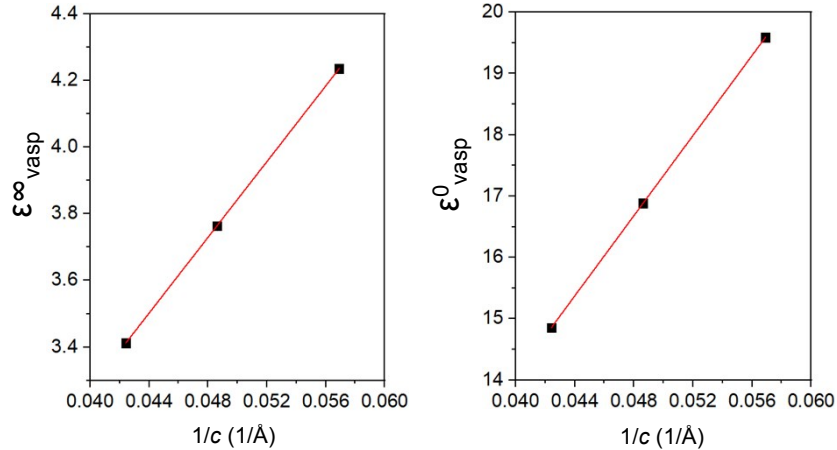
Calculation method of dielectric constants of Ba₂ZrS₄ monolayers

Because our calculation of the 2D slab includes a vacuum layer, the calculated dielectric constant from VASP (ϵ_{VASP}) is the effective one of a composite containing 2D slab and vacuum. To obtain the intrinsic value of 2D slab (ϵ_{mono}), the effective medium theory was employed. We calculated the intrinsic in-plane ϵ_{mono} by the equation [T. Sohier, *et al.*, *Physical Review B* **94**, 085415 (2016); A. Laturia, *et al.*, *npj 2D Materials and Applications* **2**, 6 (2018)]

$$\epsilon_{VASP}^{\infty} = 1 + (\epsilon_{mono}^{\infty} - 1) \frac{t}{c} \quad (1)$$

$$\epsilon_{VASP}^0 = 1 + (\epsilon_{mono}^0 - 1) \frac{t}{c} \quad (2)$$

where ϵ^{∞} and ϵ^0 are the high-frequency and static dielectric constant, respectively, t and c are thickness of the monolayer and the simulation cell along the c axis, respectively. By applying three different values of c , we calculated dielectric constant as shown in the plot below.



By fitting this data, we obtain the slope $s_1 = 56.9 \text{ \AA}$ and $s_2 = 326.9 \text{ \AA}$, respectively. We then obtain

ϵ_{mono}^{∞} and ϵ_{mono}^0 as a function of t as

$$\epsilon_{mono}^{\infty} = 1 + \frac{s_1}{t} \quad (3)$$

$$\epsilon_{mono}^0 = 1 + \frac{s_2}{t} \quad (4)$$

We used the interlayer distance in the bulk BaZrS₃ (5 Å) for the value of t .

Supplementary figures

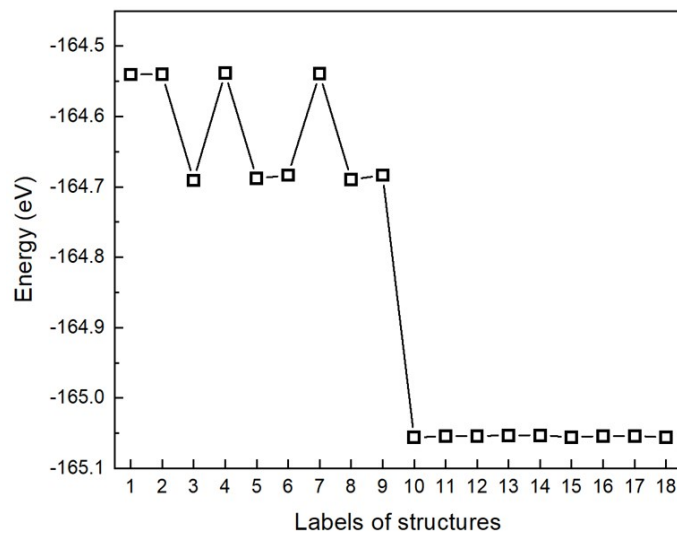


Fig. S1. Energy profile of 18 octahedral rotation patterns for the 2D perovskite Ba₂ZrS₄ ($n = 1$) after relaxation. The calculations were done by using the PBE functional.

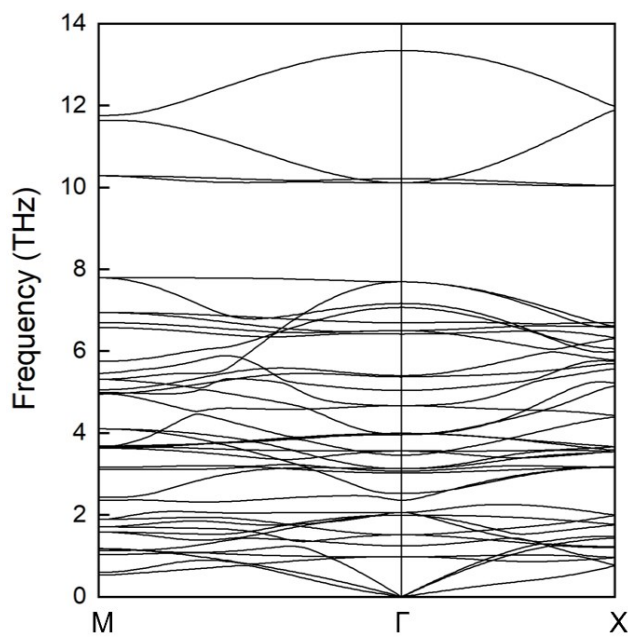


Fig. S2. Phonon spectrum of the most stable structure for Ba_2ZrS_4 ($n = 1$ with the $a^0a^0c^-$ pattern) at 300 K. The calculation was done by using the SCAN functional and the TEDP method.

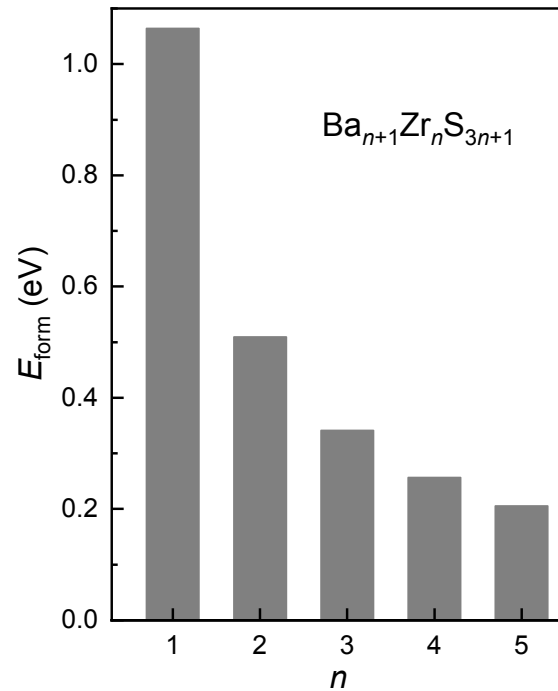


Fig. S3. Formation energy of $\text{Ba}_{n+1}\text{Zr}_n\text{S}_{3n+1}$ calculated as $E_{\text{form}} = [E_{2\text{D}} - n E_{\text{BaZrS}_3} - E_{\text{BaS}}]/n$ according to the reaction $\text{BaS} + n \text{BaZrS}_3 \rightarrow \text{Ba}_{n+1}\text{Zr}_n\text{S}_{3n+1}$.

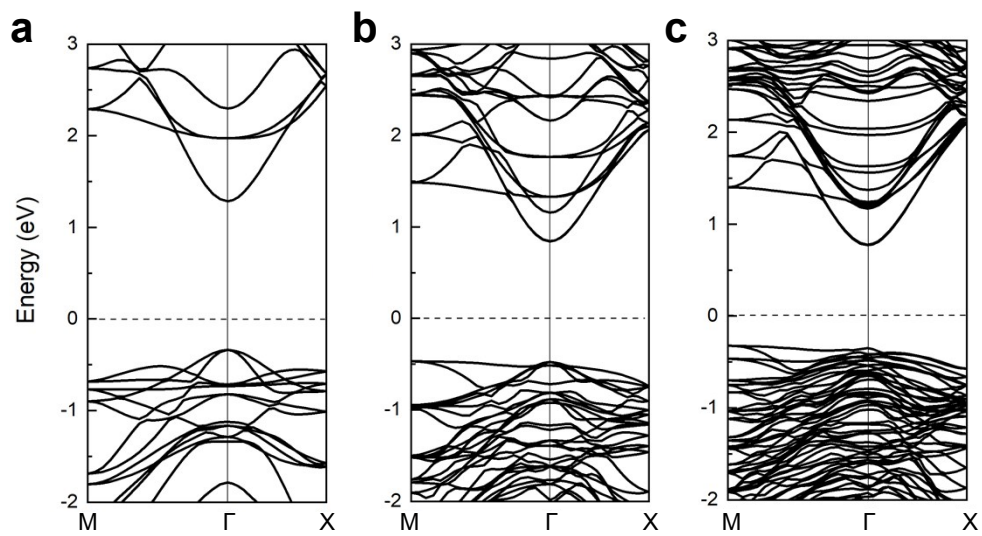


Fig. S4. Band structures of the most stable structures for $\text{Ba}_{n+1}\text{Zr}_n\text{S}_{3n+1}$ with $n = 1$ (a), 3 (b) and 5 (c).

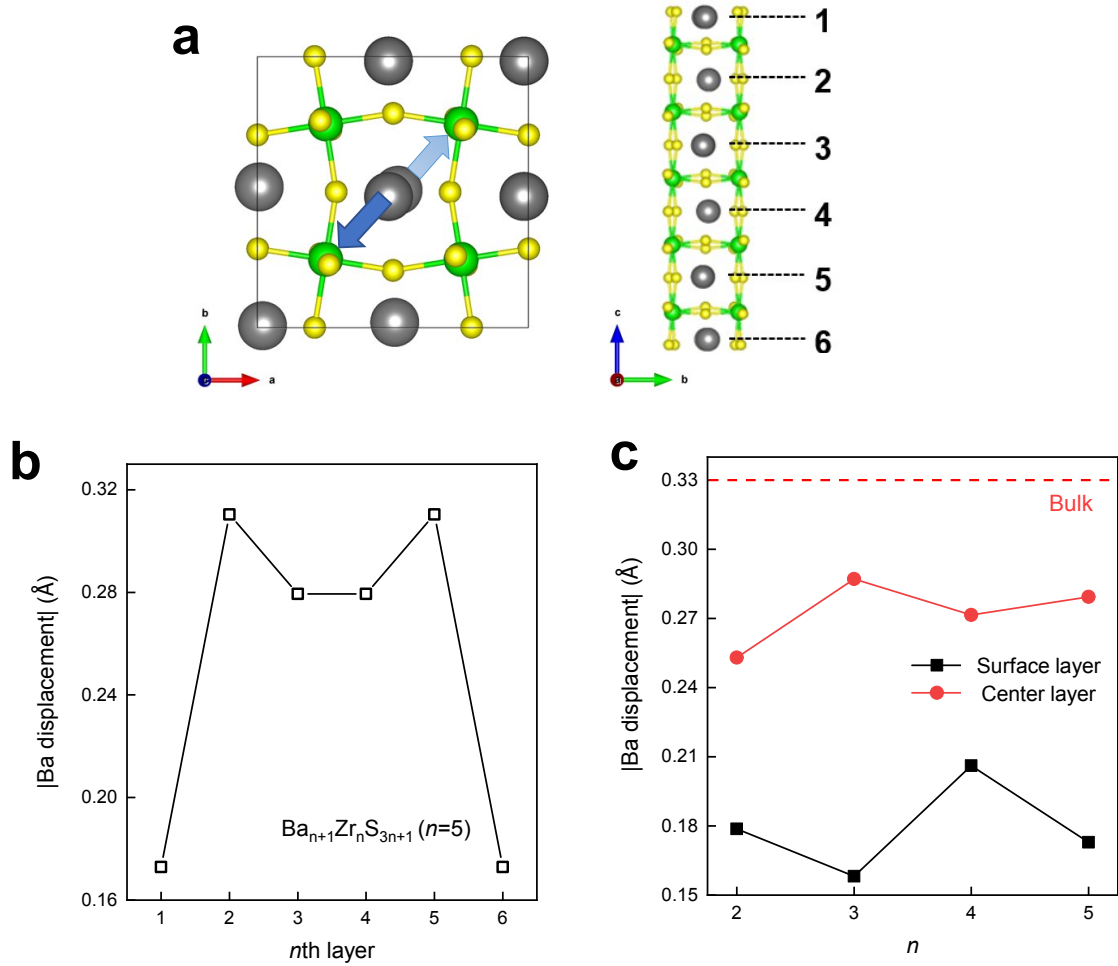


Fig. S5. Ba displacement in 2D perovskite $\text{Ba}_{n+1}\text{Zr}_n\text{S}_{3n+1}$. (a) Description of the displacement in top view (left), and side view (right) where the number indicates the layer as used in (b). (b) The magnitude of Ba displacement in each layer in 2D slab with thickness $n = 5$. (c) Evolution of the magnitude of Ba displacement in the surface and center layer with the thickness. The red dashed line indicates the magnitude in bulk BaZrS_3 .

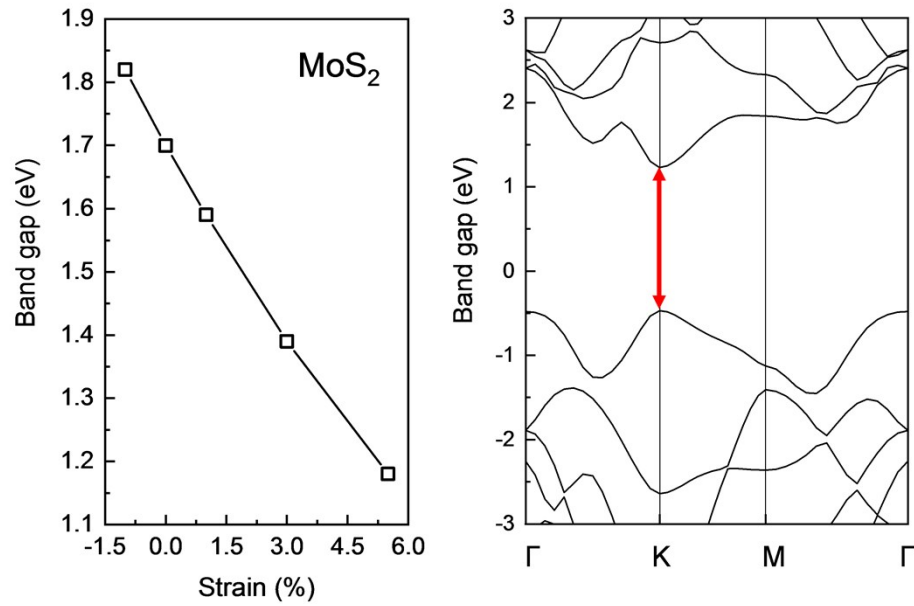


Fig. S6 (a) The direct band gap of MoS₂ as a function of the applied biaxial strain. (b) Band structure of MoS₂ at zero strain.

Supplementary tables

Table. S1. Energy of the four structures of Ba_2ZrS_4 ($n = 1$) after relaxation from 18 initial octahedral rotation patterns. The energy is relative to that of the most stable one and the unit is meV per Ba_2ZrS_4 formula unit. The calculation was performed by using the SCAN functional.

Pattern	$a^0a^0a^0$	$a^-b^0c^0$	$a^-a^-c^0$	$a^0a^0c^-$
E (meV)	122	106	107	0

Structure files

Ba₂ZrS₄ (*n*=1)

*a*⁰*a*⁰*c*⁻

1.0000000000000000

6.8092000000 0.0000000000 0.0000000000

0.0000000000 6.8092000000 0.0000000000

0.0000000000 0.0000000000 17.6079000000

Ba Zr S

4 2 8

Direct

0.500000000 0.000000000 0.640230021

0.500000000 -0.000000000 0.359770007

0.000000000 0.500000000 0.640230021

0.000000000 0.500000000 0.359770007

0.000000000 0.000000000 0.500000000

0.500000000 0.500000000 0.500000000

-0.000000000 -0.000000000 0.649280012

0.000000000 0.000000000 0.350719988

0.500000000 0.500000000 0.350719988

0.500000000 0.500000000 0.649280012

0.314440018 0.185569996 0.500000000

0.685560017 0.814430004 0.500000000

0.814430004 0.314440018 0.500000000

0.185569996 0.685560017 0.500000000

Ba₂ZrS₄ (n=1)

$a^0a^0a^0$

1.0000000000000000

9.8417959200000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.8417959200000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0671370100000000

Ba Zr S

8 4 16

Direct

0.5000000000000000	0.5000000000000000	0.3763189930434991
-0.0000000000000000	0.5000000000000000	0.3763189930434991
0.5000000000000000	0.0000000000000000	0.3763189930434991
-0.0000000000000000	0.0000000000000000	0.3763189930434991
0.5000000000000000	0.5000000000000000	0.6236810069565007
-0.0000000000000000	0.5000000000000000	0.6236810069565007
0.5000000000000000	-0.0000000000000000	0.6236810069565007
-0.0000000000000000	-0.0000000000000000	0.6236810069565007
0.2500000000000000	0.2500000000000000	0.5000000000000000
0.7500000000000000	0.2500000000000000	0.5000000000000000
0.2500000000000000	0.7500000000000000	0.5000000000000000
0.7500000000000000	0.7500000000000000	0.5000000000000000
0.2500000000000000	0.2500000000000000	0.3564109523696719
0.7500000000000000	0.2500000000000000	0.3564109523696719
0.2500000000000000	0.7500000000000000	0.3564109523696719
0.7500000000000000	0.7500000000000000	0.3564109523696719
-0.0000000000000000	0.2500000000000000	0.5000000000000000
0.2500000000000000	0.0000000000000000	0.5000000000000000

0.5000000000000000 0.2500000000000000 0.5000000000000000
 0.7500000000000000 0.0000000000000000 0.5000000000000000
 -0.0000000000000000 0.7500000000000000 0.5000000000000000
 0.2500000000000000 0.5000000000000000 0.5000000000000000
 0.5000000000000000 0.7500000000000000 0.5000000000000000
 0.7500000000000000 0.5000000000000000 0.5000000000000000
 0.2500000000000000 0.2500000000000000 0.6435890476303281
 0.7500000000000000 0.2500000000000000 0.6435890476303281
 0.2500000000000000 0.7500000000000000 0.6435890476303281
 0.7500000000000000 0.7500000000000000 0.6435890476303281

Ba₂ZrS₄ (*n*=1)

a⁻*b*⁰*c*⁰

1.0000000000000000

9.8635547300000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 9.8895308000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 17.3289702000000000

Ba Zr S

8 4 16

Direct

0.5000000000000000 0.5136627998396959 0.3720232705025357
 0.0000000000000000 0.4863372001603040 0.3720232705025357
 0.5000000000000000 0.9863372001603041 0.3720232705025357
 0.0000000000000000 0.0136627998396960 0.3720232705025357

0.5000000000000000 0.4863372001603040 0.6279767294974643
0.0000000000000000 0.5136627998396959 0.6279767294974643
0.5000000000000000 0.0136627998396960 0.6279767294974643
0.0000000000000000 0.9863372001603041 0.6279767294974643
0.2500000000000000 0.2500000000000000 0.5000000000000000
0.7500000000000000 0.2500000000000000 0.5000000000000000
0.2500000000000000 0.7500000000000000 0.5000000000000000
0.7500000000000000 0.7500000000000000 0.5000000000000000
0.2281257484002115 0.2500000000000000 0.3512255463751822
0.7718742515997956 0.2500000000000000 0.3512255463751822
0.2718742515997886 0.7500000000000000 0.3512255463751822
0.7281257484002044 0.7500000000000000 0.3512255463751822
0.0000000000000000 0.2500000000000000 0.5138825356760301
0.2500000000000000 -0.0000000000000000 0.5000000000000000
0.5000000000000000 0.2500000000000000 0.4861174643239701
0.7500000000000000 -0.0000000000000000 0.5000000000000000
0.0000000000000000 0.7500000000000000 0.4861174643239701
0.2500000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.7500000000000000 0.5138825356760301
0.7500000000000000 0.5000000000000000 0.5000000000000000
0.2718742515997886 0.2500000000000000 0.6487744536248179
0.7281257484002044 0.2500000000000000 0.6487744536248179
0.2281257484002115 0.7500000000000000 0.6487744536248179
0.7718742515997956 0.7500000000000000 0.6487744536248179

Ba₂ZrS₄ (n=1)

$\sigma\text{-}\sigma\text{-}c^0$

1.0000000000000000

9.8807285550871242 0.1206688817190235 0.0000000000000000

0.1206688817190234 9.8807285550871242 -0.0000000000000000

-0.0000000000000000 -0.0000000000000000 16.7266513870716089

Ba Zr S

8 4 16

Direct

0.7600460986695824 0.2600460986695824 0.3674912136473963

0.2600460986695824 0.7600460986695824 0.3674912136473963

0.7399544297104382 0.2399544297104382 0.6325089089637659

0.2399544297104382 0.7399544297104382 0.6325089089637659

0.7600455702895618 0.7600455702895618 0.6325089089637659

0.2600455702895618 0.2600455702895618 0.6325089089637659

0.7399539013304176 0.7399539013304176 0.3674912136473963

0.2399539013304176 0.2399539013304176 0.3674912136473963

0.5000019237279147 0.5000019237279147 0.5000001457632592

0.0000019237279147 0.0000019237279147 0.5000001457632592

0.4999980762720853 0.9999980762720853 0.5000001457632592

0.9999980762720853 0.4999980762720853 0.5000001457632592

0.5154361698501373 0.5154361698501373 0.3458856055233963

0.0154361698501372 0.0154361698501372 0.3458856055233963

0.9845635216650979 0.9845635216650979 0.6541143121777000

0.4845635216650980 0.4845635216650980 0.6541143121777000

0.5154364783349021 0.0154364783349020 0.6541143121777000

0.0154364783349020 0.5154364783349021 0.6541143121777000

0.9845638301498627 0.4845638301498629 0.3458856055233963
 0.4845638301498629 0.9845638301498627 0.3458856055233963
 0.7500000000000000 0.5000000000000000 0.5103307736507617
 0.2500000000000000 0.0000000000000000 0.5103307736507617
 0.7500000000000000 0.0000000000000000 0.4896690402737206
 0.2500000000000000 0.5000000000000000 0.4896690402737206
 0.5000000000000000 0.2500000000000000 0.4896690402737206
 0.0000000000000000 0.7500000000000000 0.4896690402737206
 0.5000000000000000 0.7500000000000000 0.5103307736507617
 0.0000000000000000 0.2500000000000000 0.5103307736507617

Ba₄Zr₂S₇ (n=2)

$a^0 a^0 c^-$

1.0000000000000000

9.7955243800000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 9.7955243800000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 22.6179268300000000

Ba Zr S

12 8 28

Direct

0.5000000000000000 0.5000000000000000 0.2826676025950405

0.0000000000000000 0.5000000000000000 0.2826676025950405
0.5000000000000000 0.0000000000000000 0.2826676025950405
0.0000000000000000 0.0000000000000000 0.2826676025950405
0.5000000000000000 0.5000000000000000 0.5000000000000000
0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.0000000000000000 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.5000000000000000 0.5000000000000000 0.7173323974049595
0.0000000000000000 0.5000000000000000 0.7173323974049595
0.5000000000000000 0.0000000000000000 0.7173323974049595
0.0000000000000000 0.0000000000000000 0.7173323974049595
0.2500000000000000 0.2500000000000000 0.3828772941722960
0.7500000000000000 0.2500000000000000 0.3828772941722960
0.2500000000000000 0.7500000000000000 0.3828772941722960
0.7500000000000000 0.7500000000000000 0.3828772941722960
0.2500000000000000 0.2500000000000000 0.6171227058277040
0.7500000000000000 0.2500000000000000 0.6171227058277040
0.2500000000000000 0.7500000000000000 0.6171227058277040
0.7500000000000000 0.7500000000000000 0.6171227058277040
0.2500000000000000 0.2500000000000000 0.2704587947897110
0.7500000000000000 0.2500000000000000 0.2704587947897110
0.2500000000000000 0.7500000000000000 0.2704587947897110
0.7500000000000000 0.7500000000000000 0.2704587947897110
0.0000000000000000 0.1967980741068303 0.3871323244510165
0.3032019258931697 0.0000000000000000 0.3871323244510165
0.5000000000000000 0.3032019258931697 0.3871323244510165
0.6967980741068303 0.0000000000000000 0.3871323244510165

0.0000000000000000 0.8032019258931697 0.3871323244510165
0.1967980741068303 0.5000000000000000 0.3871323244510165
0.5000000000000000 0.6967980741068303 0.3871323244510165
0.8032019258931697 0.5000000000000000 0.3871323244510165
0.2500000000000000 0.2500000000000000 0.5000000000000000
0.7500000000000000 0.2500000000000000 0.5000000000000000
0.2500000000000000 0.7500000000000000 0.5000000000000000
0.7500000000000000 0.7500000000000000 0.5000000000000000
0.0000000000000000 0.3032019258931697 0.6128676755489835
0.1967980741068303 0.0000000000000000 0.6128676755489835
0.5000000000000000 0.1967980741068303 0.6128676755489835
0.8032019258931697 0.0000000000000000 0.6128676755489835
0.0000000000000000 0.6967980741068303 0.6128676755489835
0.3032019258931697 0.5000000000000000 0.6128676755489835
0.5000000000000000 0.8032019258931697 0.6128676755489835
0.6967980741068303 0.5000000000000000 0.6128676755489835
0.2500000000000000 0.2500000000000000 0.7295412052102890
0.7500000000000000 0.2500000000000000 0.7295412052102890
0.2500000000000000 0.7500000000000000 0.7295412052102890
0.7500000000000000 0.7500000000000000 0.7295412052102890

Ba₄Zr₂S₇ (*n*=2)

$\sigma^- \sigma^+$

1.0000000000000000

9.9189670000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 9.9189700000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.3652583000000000

Ba Zr S

12 8 28

Direct

0.5196184612311114 0.5072211965981879 0.6124776355347379
0.0196184612311114 0.0072211965981808 0.6124776355347379
0.9844788776412443 0.9840270902932957 0.8360857142857157
0.4844788776412443 0.4840270902932957 0.8360857142857157
0.9840260187948076 0.4844799090575833 0.8360857142857157
0.4840260187948076 0.9844799090575833 0.8360857142857157
0.0072197554621241 0.5196193686132773 0.6124776072665767
0.5072197554621241 0.0196193686132773 0.6124776072665767
0.5196184612311114 0.5072211965981879 0.0596937930366934
0.0196184612311114 0.0072211965981808 0.0596937930366934
0.0072197554621241 0.5196193686132773 0.0596938213048546
0.5072197554621241 0.0196193686132773 0.0596938213048546
0.7523290247921608 0.2522453926845216 0.7137219426021773
0.2523290247921608 0.7522453926845216 0.7137219426021773
0.7522440136558046 0.7523305347700031 0.7137216371324300
0.2522440136558046 0.2523305347700031 0.7137216371324300
0.7523290247921608 0.2522453926845216 0.9584447240644920
0.2523290247921608 0.7522453926845216 0.9584447240644920
0.7522440136558046 0.7523305347700031 0.9584450295342393
0.2522440136558046 0.2523305347700031 0.9584450295342393
0.2326438424977084 0.7644987724661618 0.5961362957188570

0.7326438424977084 0.2644987724661618 0.5961362957188570
0.7720822288800022 0.2316042718439419 0.8360857142857157
0.2720822288800022 0.7316042718439419 0.8360857142857157
0.2316032485301278 0.2720834312004641 0.8360857142857157
0.7316032485301278 0.7720834312004712 0.8360857142857157
0.7644976866744244 0.7326447582520714 0.5961363266725002
0.2644976866744173 0.2326447582520643 0.5961363266725002
0.7116015890775174 0.5010828658863105 0.9442386110547218
0.2116015890775174 0.0010828658863105 0.9442386110547218
0.0010819028887497 0.7116024811730171 0.9442386075704050
0.5010819028887497 0.2116024811730242 0.9442386075704050
0.2910453066224576 0.5016433642376654 0.7091866188396736
0.7910453066224576 0.0016433642376583 0.7091866188396736
0.7116015890775174 0.5010828658863105 0.7279280556119474
0.2116015890775174 0.0010828658863105 0.7279280556119474
0.0010819028887497 0.7116024811730171 0.7279280590962642
0.5010819028887497 0.2116024811730242 0.7279280590962642
0.0016437352936833 0.2910464664958852 0.7091865350132309
0.5016437352936833 0.7910464664958852 0.7091865350132309
0.2326438424977084 0.7644987724661618 0.0760351328525743
0.7326438424977084 0.2644987724661618 0.0760351328525743
0.7644976866744244 0.7326447582520714 0.0760351018989311
0.2644976866744173 0.2326447582520643 0.0760351018989311
0.2910453066224576 0.5016433642376654 0.9629800478269956
0.7910453066224576 0.0016433642376583 0.9629800478269956
0.0016437352936833 0.2910464664958852 0.9629801316534383
0.5016437352936833 0.7910464664958852 0.9629801316534383

Ba₄Zr₃S₁₀ (n=3)

$a^0 a^0 c^-$

1.0000000000000000

9.8379828000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.8383531280000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.6498460900000000

Ba Zr S

16 12 40

Direct

0.5000000000000000	0.5000000000000000	0.2308957567719716
0.0000000000000000	0.5000000000000000	0.2309156225809872
0.5000000000000000	0.0000000000000000	0.2309081831561812
0.0000000000000000	0.0000000000000000	0.2308915383600905
0.5000000000000000	0.5000000000000000	0.4089604242112443
0.0000000000000000	0.5000000000000000	0.4089649594482196
0.5000000000000000	0.0000000000000000	0.4089627761941443
0.0000000000000000	0.0000000000000000	0.4089491442113982
0.5000000000000000	0.5000000000000000	0.5910508557886018
0.0000000000000000	0.5000000000000000	0.5910372238058557
0.5000000000000000	0.0000000000000000	0.5910350405517804
0.0000000000000000	0.0000000000000000	0.5910395757887486
0.5000000000000000	0.5000000000000000	0.7691084616399095
0.0000000000000000	0.5000000000000000	0.7690918168438188
0.5000000000000000	0.0000000000000000	0.7690843774190128
0.0000000000000000	0.0000000000000000	0.7691042432280284

0.2499968770728671 0.2499915069235215 0.3111550991253651
0.7500031229271329 0.2499915069235215 0.3111550991253651
0.2499968770728671 0.7500084930764785 0.3111550991253651
0.7500031229271329 0.7500084930764785 0.3111550991253651
0.2500000000000000 0.2500000000000000 0.5000000000000000
0.7500000000000000 0.2500000000000000 0.5000000000000000
0.2500000000000000 0.7500000000000000 0.5000000000000000
0.7500000000000000 0.7500000000000000 0.5000000000000000
0.2500031229271329 0.2500084930764785 0.6888449008746349
0.7499968770728671 0.2500084930764785 0.6888449008746349
0.2500031229271329 0.7499915069235215 0.6888449008746349
0.7499968770728671 0.7499915069235215 0.6888449008746349
0.2499997055549841 0.2500050885964740 0.2197939771443345
0.7500002944450159 0.2500050885964740 0.2197939771443345
0.2499997055549841 0.7499949114035260 0.2197939771443345
0.7500002944450159 0.7499949114035260 0.2197939771443345
0.0000000000000000 0.1988466481236415 0.3155383919716499
0.3011387445423495 0.0000000000000000 0.3155472033264317
0.5000000000000000 0.3011347154574651 0.3155393427033388
0.6988612554576505 0.0000000000000000 0.3155472033264317
0.0000000000000000 0.8011533518763585 0.3155383919716499
0.1988804319693926 0.5000000000000000 0.3155533628179583
0.5000000000000000 0.6988652845425349 0.3155393427033388
0.8011195680306074 0.5000000000000000 0.3155533628179583
0.2499975741702016 0.2500008152262367 0.4070826167660542
0.7500024258297984 0.2500008152262367 0.4070826167660542
0.2499975741702016 0.7499991847737633 0.4070826167660542

0.7500024258297984 0.7499991847737633 0.4070826167660542
0.0000000000000000 0.3041096161659098 0.5000021420135781
0.1958822589503342 0.0000000000000000 0.4999950814055367
0.5000000000000000 0.1958903838340902 0.4999978579864219
0.8041177410496658 0.0000000000000000 0.4999950814055367
0.0000000000000000 0.6958903838340902 0.5000021420135781
0.3041177410496658 0.5000000000000000 0.5000049185944633
0.5000000000000000 0.8041096161659098 0.4999978579864219
0.6958822589503342 0.5000000000000000 0.5000049185944633
0.2500024258297984 0.2499991847737633 0.5929173832339458
0.7499975741702016 0.2499991847737633 0.5929173832339458
0.2500024258297984 0.7500008152262367 0.5929173832339458
0.7499975741702016 0.7500008152262367 0.5929173832339458
0.0000000000000000 0.1988652845425349 0.6844606572966612
0.3011195680306074 0.0000000000000000 0.6844466371820417
0.5000000000000000 0.3011533518763585 0.6844616080283501
0.6988804319693926 0.0000000000000000 0.6844466371820417
0.0000000000000000 0.8011347154574651 0.6844606572966612
0.1988612554576505 0.5000000000000000 0.6844527966735683
0.5000000000000000 0.6988466481236415 0.6844616080283501
0.8011387445423495 0.5000000000000000 0.6844527966735683
0.2500002944450159 0.2499949114035260 0.7802060228556655
0.7499997055549841 0.2499949114035260 0.7802060228556655
0.2500002944450159 0.7500050885964740 0.7802060228556655
0.7499997055549841 0.7500050885964740 0.7802060228556655

Ba₄Zr₃S₁₀ (n=3)

$\sigma^- \sigma^- c^+$

1.0000000000000000

9.9852200000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.9852200000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.6462200000000000

Ba Zr S

16 12 40

Direct

0.5020716688722088	0.5165710158896075	0.2394089288235186
0.0165708060611112	0.5020745230804369	0.2394086761363472
0.5165708060611114	0.0020745230804368	0.2394086761363472
0.0020716688722088	0.0165710158896075	0.2394089288235186
0.4783093235642320	0.4811275777274545	0.4109359970692170
0.9811263021992552	0.4783105022045004	0.4109359359992104
0.4811263021992552	0.9783105022045007	0.4109359359992104
0.9783093235642318	0.9811275777274545	0.4109359970692170
0.5216906764357682	0.5188724222725455	0.5890640029307831
0.0188736978007448	0.5216894977954993	0.5890640640007896
0.5188736978007448	0.0216894977954995	0.5890640640007896
0.0216906764357680	0.0188724222725455	0.5890640029307831
0.4979283311277912	0.4834289841103924	0.7605910711764742
0.9834291939388886	0.4979254769195632	0.7605913238636526
0.4834291939388888	-0.0020745230804368	0.7605913238636526

-0.0020716688722088 0.9834289841103925 0.7605910711764742
0.2484002129331577 0.2484745132487833 0.3146092378180250
0.7484722340511383 0.2484026317872840 0.3146093361797940
0.2484722340511383 0.7484026317872841 0.3146093361797940
0.7484002129331648 0.7484745132487833 0.3146092378180250
0.2500000000000000 0.2500000000000000 0.5000000000000000
0.7500000000000000 0.2500000000000000 0.5000000000000000
0.2500000000000000 0.7500000000000000 0.5000000000000000
0.7500000000000000 0.7500000000000000 0.5000000000000000
0.2515997870668423 0.2515254867512169 0.6853907621819750
0.7515277659488617 0.2515973682127161 0.6853906638202063
0.2515277659488616 0.7515973682127159 0.6853906638202063
0.7515997870668352 0.7515254867512167 0.6853907621819750
0.2239917373921237 0.2640373220383774 0.2248084159499239
0.7640356640384486 0.2239924215904065 0.2248077071768075
0.2640356640384485 0.7239924215904066 0.2248077071768075
0.7239917373921237 0.7640373220383775 0.2248084159499239
0.9969962234085227 0.2149842664643378 0.3279903407779841
0.2778979734059766 0.9974269815405977 0.3101713965319664
0.4974229549659034 0.2778990678906873 0.3101718613334958
0.7149834939904586 0.9969943744273715 0.3279904901993876
0.9974229549659034 0.7778990678906873 0.3101718613334958
0.2149834939904585 0.4969943744273785 0.3279904901993876
0.4969962234085226 0.7149842664643377 0.3279903407779841
0.7778979734059768 0.4974269815405976 0.3101713965319664
0.2762068596292453 0.2241941529790682 0.4088474248482089
0.7241945768544567 0.2762094201175405 0.4088470040560341

0.2241945768544565 0.7762094201175406 0.4088470040560341
0.7762068596292455 0.7241941529790683 0.4088474248482089
0.9996508299910570 0.2110987872133809 0.4897185086564211
0.2889013602057123 0.0003552988091373 0.5102819197464006
0.5003491700089430 0.2889012127866191 0.5102814913435718
0.7110986397942878 0.9996447011908627 0.4897180802535994
0.0003491700089427 0.7889012127866191 0.5102814913435718
0.2110986397942878 0.4996447011908628 0.4897180802535994
0.4996508299910574 0.7110987872133809 0.4897185086564211
0.7889013602057122 0.5003552988091373 0.5102819197464006
0.2237931403707547 0.2758058470209319 0.5911525751517913
0.7758054231455433 0.2237905798824595 0.5911529959439663
0.2758054231455436 0.7237905798824594 0.5911529959439663
0.7237931403707545 0.7758058470209317 0.5911525751517913
0.0025770450340966 0.2221009321093127 0.6898281386665042
0.2850165060095416 0.0030056255726214 0.6720095098006127
0.5030037765914773 0.2850157335356622 0.6720096592220161
0.7221020265940232 0.0025730184594024 0.6898286034680337
0.0030037765914773 0.7850157335356623 0.6720096592220161
0.2221020265940233 0.5025730184594023 0.6898286034680337
0.5025770450340966 0.7221009321093127 0.6898281386665042
0.7850165060095414 0.5030056255726285 0.6720095098006127
0.2760082626078763 0.2359626779616227 0.7751915840500762
0.7359643359615514 0.2760075784095936 0.7751922928231926
0.2359643359615515 0.7760075784095934 0.7751922928231926
0.7760082626078763 0.7359626779616225 0.7751915840500762

Ba₅Zr₄S₁₃ (n=4)

a⁰a⁰c⁻

1.0000000000000000

9.8687707800000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.8687707800000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.6280952200000000

Ba Zr S

20 16 52

Direct

0.5000000000000000	0.5000000000000000	0.1938212539871485
0.0000000000000000	0.5000000000000000	0.1938212539871485
0.5000000000000000	0.0000000000000000	0.1938212539871485
0.0000000000000000	0.0000000000000000	0.1938212539871485
0.5000000000000000	0.5000000000000000	0.3446257863071416
0.0000000000000000	0.5000000000000000	0.3446257863071416
0.5000000000000000	0.0000000000000000	0.3446257863071416
0.0000000000000000	0.0000000000000000	0.3446257863071416
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.5000000000000000
0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.6553742136928585
0.0000000000000000	0.5000000000000000	0.6553742136928585
0.5000000000000000	0.0000000000000000	0.6553742136928585
0.0000000000000000	0.0000000000000000	0.6553742136928585
0.5000000000000000	0.5000000000000000	0.8061787460128514
0.0000000000000000	0.5000000000000000	0.8061787460128514

0.5000000000000000 0.0000000000000000 0.8061787460128514
0.0000000000000000 0.0000000000000000 0.8061787460128514
0.2500000000000000 0.2500000000000000 0.2612037043756372
0.7500000000000000 0.2500000000000000 0.2612037043756372
0.2500000000000000 0.7500000000000000 0.2612037043756372
0.7500000000000000 0.7500000000000000 0.2612037043756372
0.2500000000000000 0.2500000000000000 0.4209474113289599
0.7500000000000000 0.2500000000000000 0.4209474113289599
0.2500000000000000 0.7500000000000000 0.4209474113289599
0.7500000000000000 0.7500000000000000 0.4209474113289599
0.2500000000000000 0.2500000000000000 0.5790525886710403
0.7500000000000000 0.2500000000000000 0.5790525886710403
0.2500000000000000 0.7500000000000000 0.5790525886710403
0.7500000000000000 0.7500000000000000 0.5790525886710403
0.2500000000000000 0.2500000000000000 0.7387962956243624
0.7500000000000000 0.2500000000000000 0.7387962956243624
0.2500000000000000 0.7500000000000000 0.7387962956243624
0.7500000000000000 0.7500000000000000 0.7387962956243624
0.2500000000000000 0.2500000000000000 0.1839411401710803
0.7500000000000000 0.2500000000000000 0.1839411401710803
0.2500000000000000 0.7500000000000000 0.1839411401710803
0.7500000000000000 0.7500000000000000 0.1839411401710803
0.0000000000000000 0.2000184197720491 0.2651321573301761
0.2999815802279510 0.0000000000000000 0.2651321573301761
0.5000000000000000 0.2999815802279510 0.2651321573301761
0.7000184197720490 0.0000000000000000 0.2651321573301761
0.0000000000000000 0.7999815802279510 0.2651321573301761

0.2000184197720491 0.5000000000000000 0.2651321573301761
0.5000000000000000 0.7000184197720490 0.2651321573301761
0.7999815802279510 0.5000000000000000 0.2651321573301761
0.2500000000000000 0.2500000000000000 0.3425306938711327
0.7500000000000000 0.2500000000000000 0.3425306938711327
0.2500000000000000 0.7500000000000000 0.3425306938711327
0.7500000000000000 0.7500000000000000 0.3425306938711327
0.0000000000000000 0.3032124764554929 0.4215930652033730
0.1967875235445073 0.0000000000000000 0.4215930652033730
0.5000000000000000 0.1967875235445073 0.4215930652033730
0.8032124764554928 0.0000000000000000 0.4215930652033730
0.0000000000000000 0.6967875235445072 0.4215930652033730
0.3032124764554929 0.5000000000000000 0.4215930652033730
0.5000000000000000 0.8032124764554928 0.4215930652033730
0.6967875235445072 0.5000000000000000 0.4215930652033730
0.2500000000000000 0.2500000000000000 0.5000000000000000
0.7500000000000000 0.2500000000000000 0.5000000000000000
0.2500000000000000 0.7500000000000000 0.5000000000000000
0.7500000000000000 0.7500000000000000 0.5000000000000000
0.0000000000000000 0.1967875235445073 0.5784069347966270
0.3032124764554929 0.0000000000000000 0.5784069347966270
0.5000000000000000 0.3032124764554929 0.5784069347966270
0.6967875235445072 0.0000000000000000 0.5784069347966270
0.0000000000000000 0.8032124764554928 0.5784069347966270
0.1967875235445073 0.5000000000000000 0.5784069347966270
0.5000000000000000 0.6967875235445072 0.5784069347966270
0.8032124764554928 0.5000000000000000 0.5784069347966270

0.2500000000000000 0.2500000000000000 0.6574693061288669
0.7500000000000000 0.2500000000000000 0.6574693061288669
0.2500000000000000 0.7500000000000000 0.6574693061288669
0.7500000000000000 0.7500000000000000 0.6574693061288669
0.0000000000000000 0.2999815802279510 0.7348678426698243
0.2000184197720491 0.0000000000000000 0.7348678426698243
0.5000000000000000 0.2000184197720491 0.7348678426698243
0.7999815802279510 0.0000000000000000 0.7348678426698243
0.0000000000000000 0.7000184197720490 0.7348678426698243
0.2999815802279510 0.5000000000000000 0.7348678426698243
0.5000000000000000 0.7999815802279510 0.7348678426698243
0.7000184197720490 0.5000000000000000 0.7348678426698243
0.2500000000000000 0.2500000000000000 0.8160588598289197
0.7500000000000000 0.2500000000000000 0.8160588598289197
0.2500000000000000 0.7500000000000000 0.8160588598289197
0.7500000000000000 0.7500000000000000 0.8160588598289197

Ba₅Zr₄S₁₃ (n=4)

σ - σ - c^+

1.0000000000000000

10.0025900000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0025900000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.0130837000000000

Ba Zr S

20 16 52

Direct

0.4786205153193421	0.4936253929905803	0.2710652773953655
0.9786205153193421	0.9936253929905803	0.2710652773953655
0.9936250517279888	0.4786206909245649	0.2710652055417668
0.4936250517279888	0.9786206909245578	0.2710652055417668
0.0163787692039250	0.0199668560420392	0.4346231272108341
0.5163787692039179	0.5199668560420463	0.4346231272108341
0.9825921265795117	0.9767201153049285	0.6054413793103421
0.4825921265795117	0.4767201153049285	0.6054413793103421
0.9767208897582833	0.4825914718357396	0.6054413793103421
0.4767208897582833	0.9825914718357396	0.6054413793103421
0.0199669572155443	0.5163788628191099	0.4346231028302938
0.5199669572155372	0.0163788628191099	0.4346231028302938
0.0163787692039250	0.0199668560420392	0.7762596314098573
0.5163787692039179	0.5199668560420463	0.7762596314098573
0.4786205153193421	0.4936253929905803	0.9398174812253259
0.9786205153193421	0.9936253929905803	0.9398174812253259
0.9936250517279888	0.4786206909245649	0.9398175530789246
0.4936250517279888	0.9786206909245578	0.9398175530789246

0.0199669572155443 0.5163788628191099 0.7762596557903976
0.5199669572155372 0.0163788628191099 0.7762596557903976
0.2472131167650957 0.7471111421254619 0.3422436631685599
0.7472131167650886 0.2471111421254619 0.3422436631685599
0.2471107194070967 0.2472138575621372 0.3422436696508484
0.7471107194070967 0.7472138575621372 0.3422436696508484
0.2498727172541777 0.7502803943142524 0.5183422679214473
0.7498727172541777 0.2502803943142524 0.5183422679214473
0.7502801247175981 0.7498727880295561 0.5183421837792963
0.2502801247175981 0.2498727880295561 0.5183421837792963
0.2498727172541777 0.7502803943142524 0.6925370424233748
0.7498727172541777 0.2502803943142524 0.6925370424233748
0.7502801247175981 0.7498727880295561 0.6925371265655258
0.2502801247175981 0.2498727880295561 0.6925371265655258
0.2472131167650957 0.7471111421254619 0.8686356471762693
0.7472131167650886 0.2471111421254619 0.8686356471762693
0.2471107194070967 0.2472138575621372 0.8686356406939808
0.7471107194070967 0.7472138575621372 0.8686356406939808
0.7729682126339270 0.2324527556090246 0.2568364394901721
0.2729682126339270 0.7324527556090246 0.2568364394901721
0.2324523437880259 0.2729682520146639 0.2568364337207711
0.7324523437880259 0.7729682520146639 0.2568364337207711
0.7190254493120349 0.4984739918513128 0.3378459432993495
0.2190254493120349 0.9984739918513128 0.3378459432993495
0.9984740150479965 0.7190259312490568 0.3378459152220827
0.4984740150480036 0.2190259312490568 0.3378459152220827
0.2206483774100150 0.7747754101996733 0.4319975041537845

0.7206483774100079 0.2747754101996733 0.4319975041537845
0.7805191949503225 0.2229800532604571 0.6054413793103421
0.2805191949503225 0.7229800532604571 0.6054413793103421
0.2229800484953159 0.2805181526386349 0.6054413793103421
0.7229800484953159 0.7805181526386349 0.6054413793103421
0.7747753266782169 0.7206481416497326 0.4319975714368525
0.2747753266782169 0.2206481416497326 0.4319975714368525
0.7125151963159837 0.4993376867228179 0.6815958929511865
0.2125151963159837 0.9993376867228179 0.6815958929511865
0.2805260042051998 0.4991506538315917 0.3554652961369271
0.7805260042051998 0.9991506538315917 0.3554652961369271
0.9991498952470010 0.2805264572322770 0.3554652961159448
0.4991498952470010 0.7805264572322770 0.3554652961159448
0.9993375052057942 0.7125153585265522 0.6815960220868575
0.4993375052057942 0.2125153585265593 0.6815960220868575
0.2856756838101333 0.4999247243124216 0.5087648804045344
0.7856756838101333 0.9999247243124216 0.5087648804045344
0.7125151963159837 0.4993376867228179 0.5292834173936427
0.2125151963159837 0.9993376867228179 0.5292834173936427
0.9993375052057942 0.7125153585265522 0.5292832882579717
0.4993375052057942 0.2125153585265593 0.5292832882579717
0.9999245041077884 0.2856755216378417 0.5087647665825017
0.4999245041077884 0.7856755216378417 0.5087647665825017
0.2206483774100150 0.7747754101996733 0.7788852544669069
0.7206483774100079 0.2747754101996733 0.7788852544669069
0.7729682126339270 0.2324527556090246 0.9540463191305193
0.2729682126339270 0.7324527556090246 0.9540463191305193

0.2324523437880259 0.2729682520146639 0.9540463248999203
0.7324523437880259 0.7729682520146639 0.9540463248999203
0.7747753266782169 0.7206481416497326 0.7788851871838389
0.2747753266782169 0.2206481416497326 0.7788851871838389
0.2856756838101333 0.4999247243124216 0.7021144299402948
0.7856756838101333 0.9999247243124216 0.7021144299402948
0.9999245041077884 0.2856755216378417 0.7021145437623275
0.4999245041077884 0.7856755216378417 0.7021145437623275
0.2805260042051998 0.4991506538315917 0.8554140142078950
0.7805260042051998 0.9991506538315917 0.8554140142078950
0.7190254493120349 0.4984739918513128 0.8730368153213419
0.2190254493120349 0.9984739918513128 0.8730368153213419
0.9984740150479965 0.7190259312490568 0.8730368433986087
0.4984740150480036 0.2190259312490568 0.8730368433986087
0.9991498952470010 0.2805264572322770 0.8554140142288773
0.4991498952470010 0.7805264572322770 0.8554140142288773

Ba₆Zr₅S₁₆ (n=5)

a⁰a⁰c⁻

1.0000000000000000

9.8893334800000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.8893284000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	34.1777744600000000

Ba Zr S

24 20 64

Direct

0.5000000000000000	0.5000000000000000	0.1335366174274888
-0.0000000000000000	0.5000000000000000	0.1335483204513981
0.5000000000000000	-0.0000000000000000	0.1335892199259602
-0.0000000000000000	-0.0000000000000000	0.1336078105711795
0.5000000000000000	0.5000000000000000	0.2766144801220343
-0.0000000000000000	0.5000000000000000	0.2765991153747061
0.5000000000000000	-0.0000000000000000	0.2766443724170520
-0.0000000000000000	-0.0000000000000000	0.2766385252520590
0.5000000000000000	0.5000000000000000	0.4251791927083539
-0.0000000000000000	0.5000000000000000	0.4251805452792544
0.5000000000000000	-0.0000000000000000	0.4251655845815071
-0.0000000000000000	-0.0000000000000000	0.4251716351261704
0.5000000000000000	0.5000000000000000	0.5748283619595250
-0.0000000000000000	0.5000000000000000	0.5748344110150980
0.5000000000000000	-0.0000000000000000	0.5748194515146734
-0.0000000000000000	-0.0000000000000000	0.5748208072135804
0.5000000000000000	0.5000000000000000	0.7233614768018850
-0.0000000000000000	0.5000000000000000	0.7233556287167734

0.5000000000000000 -0.0000000000000000 0.7234008836989506
-0.0000000000000000 -0.0000000000000000 0.7233855268978847
0.5000000000000000 0.5000000000000000 0.8663921934856801
-0.0000000000000000 0.5000000000000000 0.8664107792424431
0.5000000000000000 -0.0000000000000000 0.8664516783386124
-0.0000000000000000 -0.0000000000000000 0.8664633888121492
0.2500212840934382 0.2500018030558406 0.1970445192066655
0.7499787159065618 0.2500018030558406 0.1970445192066655
0.2500212840934382 0.7499981969441593 0.1970445192066655
0.7499787159065618 0.7499981969441593 0.1970445192066655
0.2499783114690364 0.2500207996951546 0.3492592004306382
0.7500216885309634 0.2500207996951546 0.3492592004306382
0.2499783114690364 0.7499792003048457 0.3492592004306382
0.7500216885309634 0.7499792003048457 0.3492592004306382
0.2499999982106149 0.2500000008983611 0.5000000000370231
0.7500000017893850 0.2500000008983611 0.5000000000370231
0.2499999982106149 0.7499999991016391 0.5000000000370231
0.7500000017893850 0.7499999991016391 0.5000000000370231
0.2500216872781894 0.2499792003481957 0.6507407980409285
0.7499783127218106 0.2499792003481957 0.6507407980409285
0.2500216872781894 0.7500207996518043 0.6507407980409285
0.7499783127218106 0.7500207996518043 0.6507407980409285
0.2499787165222239 0.2499981967958946 0.8029554801781044
0.7500212834777756 0.2499981967958946 0.8029554801781044
0.2499787165222239 0.7500018032041053 0.8029554801781044
0.7500212834777756 0.7500018032041053 0.8029554801781044
0.2500814549907394 0.2499457515494386 0.1234986193305128

0.7499185450092605 0.2499457515494386 0.1234986193305128
0.2500814549907394 0.7500542484505615 0.1234986193305128
0.7499185450092605 0.7500542484505615 0.1234986193305128
-0.0000000000000000 0.2961468513427866 0.2008606324432321
0.2038664828162709 -0.0000000000000000 0.2009281909800935
0.5000000000000000 0.2038030958930848 0.2009351250744729
0.7961335171837293 -0.0000000000000000 0.2009281909800935
-0.0000000000000000 0.7038531486572135 0.2008606324432321
0.2962096429486744 0.5000000000000000 0.2008738793371087
0.5000000000000000 0.7961969041069151 0.2009351250744729
0.7037903570513323 0.5000000000000000 0.2008738793371087
0.2499365808962576 0.2500796601813009 0.2746063021134272
0.7500634191037422 0.2500796601813009 0.2746063021134272
0.2499365808962576 0.7499203398186991 0.2746063021134272
0.7500634191037422 0.7499203398186991 0.2746063021134272
-0.0000000000000000 0.1968775721881108 0.3500485439838232
0.3030575923519698 -0.0000000000000000 0.3500434680725154
0.5000000000000000 0.3030834488879129 0.3500432735407591
0.6969424076480304 -0.0000000000000000 0.3500434680725154
-0.0000000000000000 0.8031224278118964 0.3500485439838232
0.1968491613927857 0.5000000000000000 0.3500421179354052
0.5000000000000000 0.6969165511120944 0.3500432735407591
0.8031508386072145 0.5000000000000000 0.3500421179354052
0.2499274410670450 0.2500413376251564 0.4248227709930932
0.7500725589329548 0.2500413376251564 0.4248227709930932
0.2499274410670450 0.7499586623748438 0.4248227709930932
0.7500725589329548 0.7499586623748438 0.4248227709930932

-0.0000000000000000 0.3038556770514467 0.5000203613966561
0.1961485581282912 -0.0000000000000000 0.4999909195971025
0.5000000000000000 0.1961443316043554 0.4999796362169825
0.8038514418717086 -0.0000000000000000 0.4999909195971025
-0.0000000000000000 0.6961443229485531 0.5000203613966561
0.3038514373641681 0.5000000000000000 0.5000090815839343
0.5000000000000000 0.8038556683956448 0.4999796362169825
0.6961485626358319 0.5000000000000000 0.5000090815839343
0.2500725432728175 0.2499586611507474 0.5751772300929194
0.7499274567271824 0.2499586611507474 0.5751772300929194
0.2500725432728175 0.7500413388492522 0.5751772300929194
0.7499274567271824 0.7500413388492522 0.5751772300929194
-0.0000000000000000 0.1969165448393154 0.6499567290849628
0.3031508439171423 -0.0000000000000000 0.6499578810596460
0.5000000000000000 0.3031224298768448 0.6499514546251436
0.6968491560828575 -0.0000000000000000 0.6499578810596460
-0.0000000000000000 0.8030834551606775 0.6499567290849628
0.1969424002679075 0.5000000000000000 0.6499565312190949
0.5000000000000000 0.6968775701231479 0.6499514546251436
0.8030575997320926 0.5000000000000000 0.6499565312190949
0.2500634224283118 0.2499203408254790 0.7253936969522261
0.7499365775716882 0.2499203408254790 0.7253936969522261
0.2500634224283118 0.7500796591745207 0.7253936969522261
0.7499365775716882 0.7500796591745207 0.7253936969522261
-0.0000000000000000 0.2961969014648420 0.7990648731470681
0.2037903490366418 -0.0000000000000000 0.7991261255250159
0.5000000000000000 0.2038531478432062 0.7991393674428275

0.7962096509633511 -0.0000000000000000 0.7991261255250159
 -0.0000000000000000 0.7038030985351582 0.7990648731470681
 0.2961335249611998 0.5000000000000000 0.7990718119982175
 0.5000000000000000 0.7961468521567867 0.7991393674428275
 0.7038664750388002 0.5000000000000000 0.7990718119982175
 0.2499185418897154 0.2500542500578800 0.8765013787588272
 0.7500814581102777 0.2500542500578800 0.8765013787588272
 0.2499185418897154 0.7499457499421199 0.8765013787588272
 0.7500814581102777 0.7499457499421199 0.8765013787588272

Ba₆Zr₅S₁₆ (n=5)

$\sigma\sigma^c$

1.0000000000000000

10.0031500000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 10.0029500000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 32.5749900000000000

Ba Zr S

24 20 64

Direct

0.5018536862947317 0.5171277557824236 0.1251765321428982
 0.0171251747259195 0.5018714375858465 0.1251825304205580
 0.5171251754853973 0.0018714371043969 0.1251825314118077
 0.0018536859730762 0.0171277564690850 0.1251765320009318
 0.4762376167641788 0.4801979634422958 0.2709568659846681

0.9801987244540301 0.4762171640784850 0.2709587225546147
0.4801987239539643 0.9762171641035104 0.2709587224201445
0.9762376167549843 0.9801979629776931 0.2709568658584047
0.5227197341217424 0.5161004779620695 0.4233194966544529
0.0161032997033740 0.5227121751353073 0.4233190094099176
0.5161033003925010 0.0227121753148402 0.4233190096803430
0.0227197342019698 0.0161004777966693 0.4233194969772667
0.4772802658782575 0.4838995220379306 0.5766805033455471
0.9838967002966260 0.4772878248646926 0.5766809905900825
0.4838966996074990 0.9772878246851598 0.5766809903196570
0.9772802657980302 0.9838995222033307 0.5766805030227333
0.5237623832358212 0.5198020365576972 0.7290431340153319
0.0198012755459700 0.5237828359215149 0.7290412774453852
0.5198012760460357 0.0237828358964896 0.7290412775798554
0.0237623832450086 0.0198020370223069 0.7290431341415954
0.4981463137052681 0.4828722442175764 0.8748234678571019
0.9828748252740805 0.4981285624141536 0.8748174695794420
0.4828748245146026 0.9981285628956030 0.8748174685881922
0.9981463140269239 0.9828722435309150 0.8748234679990683
0.2481653104277663 0.2480504791821642 0.1886405180908264
0.7480403102832814 0.2481736309265501 0.1886411749565033
0.2480403069386858 0.7481736317291364 0.1886411742514957
0.7481653102397708 0.7480504772550020 0.1886405175189674
0.2476414734604784 0.2470144879081319 0.3453344646816831
0.7470419557436496 0.2476074010496306 0.3453360339897430
0.2470419498008976 0.7476073918213645 0.3453360303880587
0.7476414717718736 0.7470144902886205 0.3453344633848715

0.2499999957925212 0.2499999976993195 0.4999999995134132
0.7499999990049346 0.2499999982491161 0.4999999987486348
0.2500000009950654 0.7500000017508839 0.5000000012513652
0.7500000042074788 0.7500000023006805 0.5000000004865868
0.2523585282281264 0.2529855097113793 0.6546655366151214
0.7529580501991024 0.2523926081786356 0.6546639696119413
0.2529580442563504 0.7523925989503694 0.6546639660102570
0.7523585265395216 0.7529855120918681 0.6546655353183169
0.2518346897602290 0.2519495227449982 0.8113594824810326
0.7519596930613143 0.2518263682708635 0.8113588257485043
0.2519596897167184 0.7518263690734500 0.8113588250434967
0.7518346895722338 0.7519495208178356 0.8113594819091736
0.2218701468369038 0.2628195590489192 0.1125989665387972
0.7627793371828829 0.2218562592649120 0.1126000890303456
0.2627793380423554 0.7218562618678785 0.1126000887765966
0.7218701436835934 0.7628195596737066 0.1125989674223145
0.9963650870126627 0.2147348822087180 0.2003643154342850
0.2772944512669521 0.9968495141873647 0.1846883403688793
0.4968481059016867 0.2773173788515171 0.1846904290315050
0.7147224810032283 0.9963808547608363 0.2003707777606167
0.9968481039306197 0.7773173790985088 0.1846904288265702
0.2147224808420559 0.4963808542644724 0.2003707786038248
0.4963650881252659 0.7147348812468562 0.2003643153653411
0.7772944503819925 0.4968495118661070 0.1846883399201858
0.2764479127487849 0.2214085947154250 0.2685423027597194
0.7214146990281572 0.2764416376777175 0.2685418444364993
0.2214147002939465 0.7764416380509798 0.2685418435726569

0.7764479124782457 0.7214085920237114 0.2685423061237556
0.9976252919991987 0.2119706400106299 0.3367432545108923
0.2857256196976227 0.9982306568200947 0.3553929817069194
0.4982468430282976 0.2857217142589213 0.3553944695739108
0.7119790834178624 0.9976091751881412 0.3367453885851741
0.9982468402516957 0.7857217137105601 0.3553944696639650
0.2119790819279112 0.4976091759490473 0.3367453892241367
0.4976252941673630 0.7119706388504559 0.3367432540075367
0.7857256186565924 0.4982306599896837 0.3553929807012527
0.2175016165168707 0.2767691081125210 0.4228787343078338
0.7767885430407208 0.2175063371095435 0.4228788566928507
0.2767885419265257 0.7175063377356524 0.4228788566765651
0.7175016159122132 0.7767691094648118 0.4228787334254890
0.9996884432158170 0.2135580485085177 0.5094829263740009
0.2864484973165476 0.0003137910164935 0.4905220054722727
0.5003115565639787 0.2864419507215950 0.4905170734676333
0.7135515026834524 0.9996862089835065 0.5094779945277272
0.0003115567841830 0.7864419514914822 0.4905170736259991
0.2135515023672750 0.4996862091887467 0.5094779940983960
0.4996884434360213 0.7135580492784050 0.5094829265323667
0.7864484976327250 0.5003137908112533 0.4905220059016039
0.2824983840877869 0.2232308905351883 0.5771212665745180
0.7232114580734742 0.2824936622643476 0.5771211433234351
0.2232114569592794 0.7824936628904565 0.5771211433071495
0.7824983834831292 0.7232308918874789 0.5771212656921731
0.0017531597483044 0.2142782862894401 0.6446055303360351
0.2880209165821376 0.0023908248118659 0.6632546114148187

0.5023747058326370 0.2880293611495442 0.6632567459924632
0.7142743803023701 0.0017693431799053 0.6446070182930806
0.0023747080008013 0.7880293599893700 0.6632567454891076
0.2142743813434077 0.5017693400103163 0.6446070192987473
0.5017531569717022 0.7142782857410785 0.6446055304260893
0.7880209180720888 0.5023908240509528 0.6632546107758560
0.2235520875217541 0.2785914079762886 0.7314576938762444
0.7785852997060535 0.2235583619490202 0.7314581564273360
0.2785853009718428 0.7235583623222825 0.7314581555634937
0.7235520872512151 0.7785914052845750 0.7314576972402805
0.0031518960693802 0.2226826209014910 0.8153095711734297
0.2852775189967717 0.0036191452391637 0.7996292222393833
0.5036349118747411 0.2852651187531438 0.7996356846346589
0.7227055487330478 0.0031504858126280 0.8153116596311208
0.0036349129873303 0.7852651177912821 0.7996356845657150
0.2227055496180005 0.5031504881338932 0.8153116600798144
0.5031518940983134 0.7226826211484829 0.8153095709684950
0.7852775191579441 0.5036191457355276 0.7996292213961751
0.2781298563164068 0.2371804403262935 0.8874010325776854
0.7372206619576446 0.2781437381321213 0.8873999112234032
0.2372206628171172 0.7781437407350882 0.8873999109696542
0.7781298531630961 0.7371804409510807 0.8874010334612027

BaZrS₃ (Bulk)

1.0000000000000000

7.1201845163778898 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.0291027851673080 0.0000000000000000

0.0000000000000000 0.0000000000000000 10.0330181202783049

Ba Zr S

4 4 12

Direct

0.0456172701561783 0.0102675233291976 0.2500000000000000

0.9543827298438217 0.9897324766708024 0.7500000000000000

0.4543827298438217 0.5102675233291976 0.7500000000000000

0.5456172701561783 0.4897324766708024 0.2500000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.5000000000000000

0.5000000000000000 0.0000000000000000 0.5000000000000000

0.9944497973690716 0.5619906380515260 0.2500000000000000

0.0055502026309284 0.4380093619484740 0.7500000000000000

0.5055502026309284 0.0619906380515260 0.7500000000000000

0.4944497973690716 0.9380093619484740 0.2500000000000000

0.2105910109902140 0.7895150801291280 0.9683136415205098

0.7894089890097788 0.2104849198708720 0.0316863584794902

0.2894089890097860 0.2895150801291280 0.0316863584794902

0.7105910109902212 0.7104849198708720 0.9683136415205098

0.7894089890097788 0.2104849198708720 0.4683136415205098

0.2105910109902140 0.7895150801291280 0.5316863584794902

0.7105910109902212 0.7104849198708720 0.5316863584794902

0.2894089890097860 0.2895150801291280 0.4683136415205098

Ba₂ZrS₄ ($n=1, a^0a^0c^-$) 1.1% strain

1.0000000000000000

6.8840000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.8840000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000	0.0000000000000000	0.6384239664934140
0.5000000000000000	0.0000000000000000	0.3615760335065862
-0.0000000000000000	0.5000000000000000	0.6384239664934140
-0.0000000000000000	0.5000000000000000	0.3615760335065862
-0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
-0.0000000000000000	0.0000000000000000	0.6491991507936810
-0.0000000000000000	0.0000000000000000	0.3508008492063189
0.5000000000000000	0.5000000000000000	0.3508008492063189
0.5000000000000000	0.5000000000000000	0.6491991507936810
0.3082663255388813	0.1917336744611186	0.5000000000000000
0.6917336744611186	0.8082663255388814	0.5000000000000000
0.8082663255388814	0.3082663255388813	0.5000000000000000
0.1917336744611186	0.6917336744611186	0.5000000000000000

Ba₂ZrS₄ (*n*=1, *a*⁰*a*⁰*c*⁻) 2.2% strain

1.0000000000000000

6.9590000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 6.9590000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000 0.0000000000000000 0.6353491295546125

0.5000000000000000 0.0000000000000000 0.3646508704453876

-0.0000000000000000 0.5000000000000000 0.6353491295546125

-0.0000000000000000 0.5000000000000000 0.3646508704453876

-0.0000000000000000 0.0000000000000000 0.5000000000000000

0.5000000000000000 0.5000000000000000 0.5000000000000000

-0.0000000000000000 0.0000000000000000 0.6484439582494966

-0.0000000000000000 0.0000000000000000 0.3515560417505031

0.5000000000000000 0.5000000000000000 0.3515560417505031

0.5000000000000000 0.5000000000000000 0.6484439582494966

0.3004851872929433 0.1995148127070567 0.5000000000000000

0.6995148127070570 0.8004851872929430 0.5000000000000000

0.8004851872929430 0.3004851872929433 0.5000000000000000

0.1995148127070567 0.6995148127070570 0.5000000000000000

Ba₂ZrS₄ (*n*=1, *a*⁰*a*⁰*c*⁻) 3.3% strain

1.0000000000000000

7.0340000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0340000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000	0.0000000000000000	0.6326728339176102
0.5000000000000000	0.0000000000000000	0.3673271660823897
-0.0000000000000000	0.5000000000000000	0.6326728339176102
-0.0000000000000000	0.5000000000000000	0.3673271660823897
-0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
-0.0000000000000000	0.0000000000000000	0.6476699261555313
-0.0000000000000000	0.0000000000000000	0.3523300738444686
0.5000000000000000	0.5000000000000000	0.3523300738444685
0.5000000000000000	0.5000000000000000	0.6476699261555313
0.2944980586491540	0.2055019413508461	0.5000000000000000
0.7055019413508462	0.7944980586491538	0.5000000000000000
0.7944980586491538	0.2944980586491540	0.5000000000000000
0.2055019413508461	0.7055019413508462	0.5000000000000000

Ba₂ZrS₄ (*n*=1, *a*⁰*a*⁰*c*⁻) 4.4% strain

1.0000000000000000

7.1090000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.1090000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000 -0.0000000000000000 0.6285729596247013

0.5000000000000000 -0.0000000000000000 0.3714270403752984

-0.0000000000000000 0.5000000000000000 0.6285729596247013

-0.0000000000000000 0.5000000000000000 0.3714270403752984

-0.0000000000000000 -0.0000000000000000 0.5000000000000000

0.5000000000000000 0.5000000000000000 0.5000000000000000

-0.0000000000000000 -0.0000000000000000 0.6468245411324199

-0.0000000000000000 -0.0000000000000000 0.3531754588675798

0.5000000000000000 0.5000000000000000 0.3531754588675798

0.5000000000000000 0.5000000000000000 0.6468245411324199

0.2821961421155388 0.2178038578844610 0.5000000000000000

0.7178038578844610 0.7821961421155390 0.5000000000000000

0.7821961421155390 0.2821961421155388 0.5000000000000000

0.2178038578844610 0.7178038578844610 0.5000000000000000

Ba₂ZrS₄ (*n*=1, *a*⁰*a*⁰*c*⁻) 5.5% strain

1.0000000000000000

7.1840000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.1840000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000 0.0000000000000000 0.6243990516948961

0.5000000000000000 0.0000000000000000 0.3756009483051040

-0.0000000000000000 0.5000000000000000 0.6243990516948961

-0.0000000000000000 0.5000000000000000 0.3756009483051040

-0.0000000000000000 0.0000000000000000 0.5000000000000000

0.5000000000000000 0.5000000000000000 0.5000000000000000

-0.0000000000000000 0.0000000000000000 0.6460947247395877

-0.0000000000000000 0.0000000000000000 0.3539052752604122

0.5000000000000000 0.5000000000000000 0.3539052752604122

0.5000000000000000 0.5000000000000000 0.6460947247395877

0.2649820323011392 0.2350179676988608 0.5000000000000000

0.7350179676988610 0.7649820323011390 0.5000000000000000

0.7649820323011390 0.2649820323011392 0.5000000000000000

0.2350179676988608 0.7350179676988610 0.5000000000000000

Ba₂ZrS₄ (n=1, a⁰a⁰c⁻) 6.6% strain

1.0000000000000000

7.2590000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.2590000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.5000000000000000

Ba Zr S

4 2 8

Direct

0.5000000000000000 0.0000000000000000 0.6224140912289808

0.5000000000000000 0.0000000000000000 0.3775859087710191

0.0000000000000000 0.5000000000000000 0.6224140912289808

0.0000000000000000 0.5000000000000000 0.3775859087710191

0.0000000000000000 0.0000000000000000 0.5000000000000000

0.5000000000000000 0.5000000000000000 0.5000000000000000

0.0000000000000000 0.0000000000000000 0.6453465156500909

0.0000000000000000 0.0000000000000000 0.3546534843499088

0.5000000000000000 0.5000000000000000 0.3546534843499088

0.5000000000000000 0.5000000000000000 0.6453465156500909

0.2594814497636668 0.2405185502363332 0.5000000000000000

0.7405185502363334 0.7594814497636666 0.5000000000000000

0.7594814497636666 0.2594814497636668 0.5000000000000000

0.2405185502363332 0.7405185502363334 0.5000000000000000