

## Negative linear compressibility from helix in zinc carbodiimide

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### Computational details

The First-principles calculation were performed by The Vienna Ab initio Simulation Package (VASP)<sup>1</sup>, a plane-wave pseudopotential total energy package based on density functional theory (DFT). The projector augmented wave (PAW) pseudopotential were used to model the effective interaction between the valence electrons and atom cores, which allow us to use a small plane basis set without compromising the accuracy required by the calculation. The functionals developed by Perdew-Burke-Ernzerhof (PBE) in generalized gradient approximation (GGA) form were adopted to describe the exchange-correlation energy.<sup>1-4</sup> A plane-wave basis set was used with an energy cutoff of 600 eV in all calculations, obtained as good values from convergence tests. K-point sampling was performed using no less than 3×3×6 mesh-Monkhorst pack scheme for Zn(CN<sub>2</sub>), and the structures were fully optimized until the maximum energy and force were less than 10<sup>-6</sup> eV and 0.001 eV/Å. The vibrational property was calculated by supercell and finite displacement approaches with a 2×2×2 supercell (128 atoms) of the primitive cell with the PHONOPY code. AIMD simulations were performed in the NPT ensemble applying a Nose'-Hoover thermostat combined with a supercell method (256 atoms for Zn(CN<sub>2</sub>)) with G point for Brillouin zone sampling to determine dynamical properties at high temperatures. Crystal structures and the electron localization function (ELF) were plotted using vesta software.

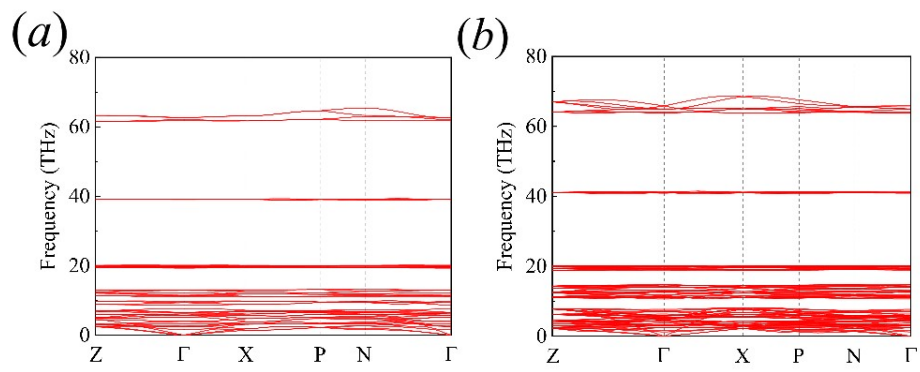


Figure S1. Phonon dispersion at 0 GPa (a) and 10 GPa (b) for Zn(CN<sub>2</sub>).



Figure S2. Calculated eigenvectors of selected phonon modes in 30.9 meV at the gamma point.

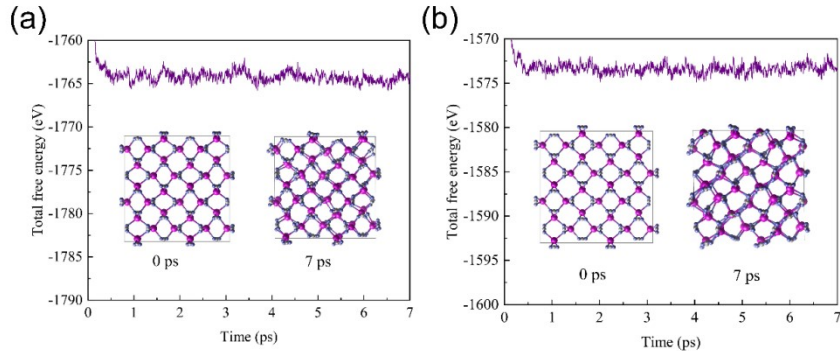


Fig. S3 The total free energy of  $\text{Zn}(\text{CN}_2)$  as a function of AIMD simulation time at 300 K under (a) 0 GPa and (b) 10 GPa. The inset presents the structure snapshots of  $\text{Zn}(\text{CN}_2)$  at 0 and 7 ps, respectively.

Table S1. Comparison of calculated and experimental lattice parameters and  $K_c$  of  $\text{Zn}(\text{CN}_2)$ .

	0 GPa		10 GPa		$K_c$ ( $\text{TPa}^{-1}$ )
	a ( $\text{\AA}$ )	c ( $\text{\AA}$ )	a ( $\text{\AA}$ )	c ( $\text{\AA}$ )	
Expt. <sup>5</sup>	8.8047	5.4329	-	-	-
CA (LDA)	8.5372	5.4321	7.6341	5.7022	-4.97
pw91 (GGA)	8.9903	5.4021	8.0297	5.6817	-5.19
PBE (GGA)	8.8150	5.4567	7.8548	5.7457	-5.29
DFT-D2	8.6591	5.5307	7.7530	5.7779	-4.46
DFT-D3	8.8429	5.4499	7.7055	5.7814	-6.08
DFT-D3(BJ)	8.5655	5.5382	7.6233	5.8204	-5.09
DFT-D4	8.8195	5.4590	7.8518	5.7467	-5.31
DFT-TS	8.6362	5.5039	7.7754	5.7501	-4.47
DFT-TS/HI	8.9135	5.4042	7.8824	5.726	-5.95
DFT-dDsC	8.7935	5.4532	7.7759	5.7659	-5.73
DFT-MBD@rSC	8.8224	5.4467	7.8363	5.7409	-5.40

Table S2. The calculated elastic constants  $C_{ij}$  at 0 GPa and compressibilities calculated based on elastic constants.

$C_{11}$	$C_{12}$	$C_{13}$	$C_{33}$	$C_{44}$	$C_{66}$	$K_a(\text{TPa}^{-1})$	$K_c(\text{TPa}^{-1})$
68.78	40.12	80.65	208.60	22.48	27.95	-5.4	13.2

Table S3. The average lattice parameters of  $\text{Zn}(\text{CN}_2)$  ( $2 \times 2 \times 2$  supercell)

	a (Å)	b (Å)	c (Å)
0 GPa	16.6442	16.7135	10.7008
10 GPa	14.8398	14.9156	11.2536

**Table S2.** Energies of  $\text{Zn}(\text{CN}_2)$  under different pressure.

Pressure (GPa)	Energy (eV)
0	-222.59265844
1	-219.96595054
2	-217.38783679
3	-214.85846347
4	-212.37725853
5	-209.94279851
6	-207.55409085
7	-205.20980456
8	-202.90883818
9	-200.64818737
10	-198.43306292

Table S5. Atom coordinates of Zn(CN<sub>2</sub>) under different pressure.

0GPa

```

1.0000000000000000
  8.8224278108859675    0.0000000000000000    0.0000000000000000
  0.0000000000000000    8.8224278108859675    0.0000000000000000
  0.0000000000000000    0.0000000000000000    5.4467182357641564
  
```

```

N    Zn    C
 16     8     8
  
```

Direct

```

0.8088252255012662  0.4271591189174799  0.0798958386700335
0.1911747894987315  0.5728408810825201  0.0798958386700335
0.4271591189174799  0.1911747894987315  0.9201041613299665
0.5728408810825201  0.8088252255012662  0.9201041613299665
0.6911747744987338  0.4271591189174799  0.6701041613299665
0.3088252255012662  0.5728408810825201  0.6701041613299665
0.0728408810825201  0.1911747894987315  0.8298958386700335
0.9271591189174799  0.8088252255012662  0.8298958386700335
0.3088252255012662  0.9271591189174799  0.5798958386700335
0.6911747744987338  0.0728408810825201  0.5798958386700335
0.9271591189174799  0.6911747744987338  0.4201041613299665
0.0728408810825201  0.3088252255012662  0.4201041613299665
0.1911747894987315  0.9271591189174799  0.1701041613299665
0.8088252255012662  0.0728408810825201  0.1701041613299665
0.5728408810825201  0.6911747744987338  0.3298958386700335
0.4271591189174799  0.3088252255012662  0.3298958386700335
0.4547730888606054  0.7500000000000000  0.6250000000000000
0.5452269111393946  0.2500000000000000  0.6250000000000000
0.7500000000000000  0.5452269111393946  0.3750000000000000
0.2500000000000000  0.4547730888606054  0.3750000000000000
0.0452269111393946  0.7500000000000000  0.1250000000000000
0.9547730888606054  0.2500000000000000  0.1250000000000000
0.2500000000000000  0.0452269111393946  0.8750000000000000
0.7500000000000000  0.9547730888606054  0.8750000000000000
0.2500000000000000  0.9311721232053998  0.3750000000000000
0.7500000000000000  0.0688278847946009  0.3750000000000000
0.9311721232053998  0.7500000000000000  0.6250000000000000
0.0688278847946009  0.2500000000000000  0.6250000000000000
0.5688278767946002  0.7500000000000000  0.1250000000000000
0.4311721232053998  0.2500000000000000  0.1250000000000000
0.7500000000000000  0.4311721232053998  0.8750000000000000
0.2500000000000000  0.5688278767946002  0.8750000000000000
  
```

1GPa

1.000000000000000		
8.7141969887517785	0.000000000000000	0.000000000000000
0.000000000000000	8.7141969887517785	0.000000000000000
0.000000000000000	0.000000000000000	5.4773461440391920

N	Zn	C
16	8	8

Direct

0.8076738516349593	0.4292677077132865	0.0798691868337897
0.1923261633650384	0.5707322922867135	0.0798691868337897
0.4292677077132865	0.1923261633650384	0.9201308131662103
0.5707322922867135	0.8076738516349593	0.9201308131662103
0.6923261483650407	0.4292677077132865	0.6701308131662103
0.3076738516349593	0.5707322922867135	0.6701308131662103
0.0707322922867135	0.1923261633650384	0.8298691868337897
0.9292677077132865	0.8076738516349593	0.8298691868337897
0.3076738516349593	0.9292677077132865	0.5798691868337897
0.6923261483650407	0.0707322922867135	0.5798691868337897
0.9292677077132865	0.6923261483650407	0.4201308131662103
0.0707322922867135	0.3076738516349593	0.4201308131662103
0.1923261633650384	0.9292677077132865	0.1701308131662103
0.8076738516349593	0.0707322922867135	0.1701308131662103
0.5707322922867135	0.6923261483650407	0.3298691868337897
0.4292677077132865	0.3076738516349593	0.3298691868337897
0.4541342101568446	0.750000000000000	0.625000000000000
0.5458657898431554	0.250000000000000	0.625000000000000
0.750000000000000	0.5458657898431554	0.375000000000000
0.250000000000000	0.4541342101568446	0.375000000000000
0.0458657898431554	0.750000000000000	0.125000000000000
0.9541342101568446	0.250000000000000	0.125000000000000
0.250000000000000	0.0458657898431554	0.875000000000000
0.750000000000000	0.9541342101568446	0.875000000000000
0.250000000000000	0.9337662136435156	0.375000000000000
0.750000000000000	0.0662337943564850	0.375000000000000
0.9337662136435156	0.750000000000000	0.625000000000000
0.0662337943564850	0.250000000000000	0.625000000000000
0.5662337863564844	0.750000000000000	0.125000000000000
0.4337662136435156	0.250000000000000	0.125000000000000
0.750000000000000	0.4337662136435156	0.875000000000000
0.250000000000000	0.5662337863564844	0.875000000000000

2GPa

1.000000000000000		
8.6098823418196755	0.000000000000000	0.000000000000000
0.000000000000000	8.6098823418196755	0.000000000000000
0.000000000000000	0.000000000000000	5.5069769171220564

N	Zn	C
16	8	8

Direct

0.8066520665200940	0.4315121138291502	0.0797076886891475
0.1933479484799037	0.5684878861708498	0.0797076886891475
0.4315121138291502	0.1933479484799037	0.9202923113108525
0.5684878861708498	0.8066520665200940	0.9202923113108525
0.6933479334799060	0.4315121138291502	0.6702923113108525
0.3066520665200940	0.5684878861708498	0.6702923113108525
0.0684878861708498	0.1933479484799037	0.8297076886891475
0.9315121138291502	0.8066520665200940	0.8297076886891475
0.3066520665200940	0.9315121138291502	0.5797076886891475
0.6933479334799060	0.0684878861708498	0.5797076886891475
0.9315121138291502	0.6933479334799060	0.4202923113108525
0.0684878861708498	0.3066520665200940	0.4202923113108525
0.1933479484799037	0.9315121138291502	0.1702923113108525
0.8066520665200940	0.0684878861708498	0.1702923113108525
0.5684878861708498	0.6933479334799060	0.3297076886891475
0.4315121138291502	0.3066520665200940	0.3297076886891475
0.4534663322465491	0.750000000000000	0.625000000000000
0.5465336677534509	0.250000000000000	0.625000000000000
0.750000000000000	0.5465336677534509	0.375000000000000
0.250000000000000	0.4534663322465491	0.375000000000000
0.0465336677534509	0.750000000000000	0.125000000000000
0.9534663322465491	0.250000000000000	0.125000000000000
0.250000000000000	0.0465336677534509	0.875000000000000
0.750000000000000	0.9534663322465491	0.875000000000000
0.250000000000000	0.9364865853999831	0.375000000000000
0.750000000000000	0.0635134226000176	0.375000000000000
0.9364865853999831	0.750000000000000	0.625000000000000
0.0635134226000176	0.250000000000000	0.625000000000000
0.5635134146000169	0.750000000000000	0.125000000000000
0.4364865853999831	0.250000000000000	0.125000000000000
0.750000000000000	0.4364865853999831	0.875000000000000
0.250000000000000	0.5635134146000169	0.875000000000000

3GPa

1.0000000000000000		
8.5046996656368918	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5046996656368918	-0.0000000000000000
0.0000000000000000	-0.0000000000000000	5.5385547592047919

N	Zn	C
16	8	8

Direct

0.8054568878687647	0.4338792842179705	0.0795428040436465
0.1945431271312330	0.5661207157820294	0.0795428040436465
0.4338792842179705	0.1945431271312330	0.9204571959563536
0.5661207157820294	0.8054568878687647	0.9204571959563536
0.6945431121312353	0.4338792842179705	0.6704571959563536
0.3054568878687646	0.5661207157820294	0.6704571959563536
0.0661207157820295	0.1945431271312330	0.8295428040436464
0.9338792842179706	0.8054568878687647	0.8295428040436464
0.3054568878687646	0.9338792842179706	0.5795428040436464
0.6945431121312353	0.0661207157820295	0.5795428040436464
0.9338792842179706	0.6945431121312353	0.4204571959563536
0.0661207157820295	0.3054568878687646	0.4204571959563536
0.1945431271312330	0.9338792842179706	0.1704571959563535
0.8054568878687647	0.0661207157820295	0.1704571959563535
0.5661207157820294	0.6945431121312353	0.3295428040436464
0.4338792842179705	0.3054568878687646	0.3295428040436464
0.4527265612026653	0.7500000000000000	0.6250000000000000
0.5472734387973348	0.2500000000000000	0.6250000000000000
0.7500000000000000	0.5472734387973348	0.3750000000000000
0.2500000000000000	0.4527265612026653	0.3750000000000000
0.0472734387973347	0.7500000000000000	0.1250000000000000
0.9527265612026652	0.2500000000000000	0.1250000000000000
0.2500000000000000	0.0472734387973347	0.8750000000000000
0.7500000000000000	0.9527265612026652	0.8750000000000000
0.2500000000000000	0.9393651344943951	0.3750000000000000
0.7500000000000000	0.0606348735056055	0.3750000000000000
0.9393651344943951	0.7500000000000000	0.6250000000000000
0.0606348735056055	0.2500000000000000	0.6250000000000000
0.5606348655056049	0.7500000000000000	0.1250000000000000
0.4393651344943952	0.2500000000000000	0.1250000000000000
0.7500000000000000	0.4393651344943952	0.8750000000000000
0.2500000000000000	0.5606348655056049	0.8750000000000000



4GPa

1.000000000000000		
8.4020102377648271	0.000000000000000	0.000000000000000
0.000000000000000	8.4020102377648271	0.000000000000000
0.000000000000000	0.000000000000000	5.5697738694302261

N	Zn	C
16	8	8

Direct

0.8041616501134925	0.4363527321876290	0.0793840429101635
0.1958383648865052	0.5636472678123639	0.0793840429101635
0.4363527321876290	0.1958383648865052	0.9206159570898365
0.5636472678123639	0.8041616501134925	0.9206159570898365
0.6958383498865075	0.4363527321876290	0.6706159570898365
0.3041616501134925	0.5636472678123639	0.6706159570898365
0.0636472678123710	0.1958383648865052	0.8293840429101635
0.9363527321876361	0.8041616501134925	0.8293840429101635
0.3041616501134925	0.9363527321876361	0.5793840429101635
0.6958383498865075	0.0636472678123710	0.5793840429101635
0.9363527321876361	0.6958383498865075	0.4206159570898365
0.0636472678123710	0.3041616501134925	0.4206159570898365
0.1958383648865052	0.9363527321876361	0.1706159570898365
0.8041616501134925	0.0636472678123710	0.1706159570898365
0.5636472678123639	0.6958383498865075	0.3293840429101635
0.4363527321876290	0.3041616501134925	0.3293840429101635
0.4518238886860431	0.750000000000000	0.625000000000000
0.5481761113139569	0.250000000000000	0.625000000000000
0.750000000000000	0.5481761113139569	0.375000000000000
0.250000000000000	0.4518238886860431	0.375000000000000
0.0481761113139569	0.750000000000000	0.125000000000000
0.9518238886860431	0.250000000000000	0.125000000000000
0.250000000000000	0.0481761113139569	0.875000000000000
0.750000000000000	0.9518238886860431	0.875000000000000
0.250000000000000	0.9423727176357488	0.375000000000000
0.750000000000000	0.0576272903642518	0.375000000000000
0.9423727176357488	0.750000000000000	0.625000000000000
0.0576272903642518	0.250000000000000	0.625000000000000
0.5576272823642512	0.750000000000000	0.125000000000000
0.4423727176357488	0.250000000000000	0.125000000000000
0.750000000000000	0.4423727176357488	0.875000000000000
0.250000000000000	0.5576272823642512	0.875000000000000

5GPa

1.000000000000000		
8.2987433050108361	0.000000000000000	0.000000000000000
0.000000000000000	8.2987433050108024	0.000000000000000
0.000000000000000	0.000000000000000	5.6021389431935500

N	Zn	C
16	8	8

Direct

0.8026330580669239	0.4390909097478968	0.0792594696138025
0.1973669569330738	0.5609090902521032	0.0792594696138025
0.4390909097478968	0.1973669569330738	0.9207405303861975
0.5609090902521032	0.8026330580669239	0.9207405303861975
0.6973669419330761	0.4390909097478968	0.6707405303861975
0.3026330580669239	0.5609090902521032	0.6707405303861975
0.0609090902521032	0.1973669569330738	0.8292594696138025
0.9390909097478968	0.8026330580669239	0.8292594696138025
0.3026330580669239	0.9390909097478968	0.5792594696138025
0.6973669419330761	0.0609090902521032	0.5792594696138025
0.9390909097478968	0.6973669419330761	0.4207405303861975
0.0609090902521032	0.3026330580669239	0.4207405303861975
0.1973669569330738	0.9390909097478968	0.1707405303861975
0.8026330580669239	0.0609090902521032	0.1707405303861975
0.5609090902521032	0.6973669419330761	0.3292594696138025
0.4390909097478968	0.3026330580669239	0.3292594696138025
0.4505871044136711	0.750000000000000	0.625000000000000
0.5494128955863289	0.250000000000000	0.625000000000000
0.750000000000000	0.5494128955863289	0.375000000000000
0.250000000000000	0.4505871044136711	0.375000000000000
0.0494128955863289	0.750000000000000	0.125000000000000
0.9505871044136711	0.250000000000000	0.125000000000000
0.250000000000000	0.0494128955863289	0.875000000000000
0.750000000000000	0.9505871044136711	0.875000000000000
0.250000000000000	0.9457073078271989	0.375000000000000
0.750000000000000	0.0542927001728017	0.375000000000000
0.9457073078271989	0.750000000000000	0.625000000000000
0.0542927001728017	0.250000000000000	0.625000000000000
0.5542926921728011	0.750000000000000	0.125000000000000
0.4457073078271989	0.250000000000000	0.125000000000000
0.750000000000000	0.4457073078271989	0.875000000000000
0.250000000000000	0.5542926921728011	0.875000000000000

6GPa

1.000000000000000		
8.1958530754794765	0.000000000000000	0.000000000000000
0.000000000000000	8.1958530754794765	0.000000000000000
0.000000000000000	0.000000000000000	5.6350210135778855

N	Zn	C
16	8	8

Direct

0.8008565298414041	0.4419355539354939	0.0791737680472622
0.1991434851585936	0.5580644460645061	0.0791737680472622
0.4419355539354939	0.1991434851585936	0.9208262319527378
0.5580644460645061	0.8008565298414041	0.9208262319527378
0.6991434701585959	0.4419355539354939	0.6708262319527378
0.3008565298414041	0.5580644460645061	0.6708262319527378
0.0580644460645061	0.1991434851585936	0.8291737680472622
0.9419355539354939	0.8008565298414041	0.8291737680472622
0.3008565298414041	0.9419355539354939	0.5791737680472622
0.6991434701585959	0.0580644460645061	0.5791737680472622
0.9419355539354939	0.6991434701585959	0.4208262319527378
0.0580644460645061	0.3008565298414041	0.4208262319527378
0.1991434851585936	0.9419355539354939	0.1708262319527378
0.8008565298414041	0.0580644460645061	0.1708262319527378
0.5580644460645061	0.6991434701585959	0.3291737680472622
0.4419355539354939	0.3008565298414041	0.3291737680472622
0.4491489010858061	0.750000000000000	0.625000000000000
0.5508510989142010	0.250000000000000	0.625000000000000
0.750000000000000	0.5508510989142010	0.375000000000000
0.250000000000000	0.4491489010858061	0.375000000000000
0.0508510989141939	0.750000000000000	0.125000000000000
0.9491489010857990	0.250000000000000	0.125000000000000
0.250000000000000	0.0508510989141939	0.875000000000000
0.750000000000000	0.9491489010857990	0.875000000000000
0.250000000000000	0.9491961470749928	0.375000000000000
0.750000000000000	0.0508038609250079	0.375000000000000
0.9491961470749928	0.750000000000000	0.625000000000000
0.0508038609250079	0.250000000000000	0.625000000000000
0.5508038529250072	0.750000000000000	0.125000000000000
0.4491961470749928	0.250000000000000	0.125000000000000
0.750000000000000	0.4491961470749928	0.875000000000000
0.250000000000000	0.5508038529250072	0.875000000000000

7GPa

1.000000000000000		
8.0983654660467757	0.000000000000000	0.000000000000000
0.000000000000000	8.0983654660467757	0.000000000000000
0.000000000000000	0.000000000000000	5.6654636421374631

N	Zn	C
16	8	8

Direct

0.7992777284036094	0.4448257350947955	0.0789885395572867
0.2007222865963882	0.5551742649052045	0.0789885395572867
0.4448257350947955	0.2007222865963882	0.9210114604427133
0.5551742649052045	0.7992777284036094	0.9210114604427133
0.7007222715963906	0.4448257350947955	0.6710114604427133
0.2992777284036094	0.5551742649052045	0.6710114604427133
0.0551742649052045	0.2007222865963882	0.8289885395572867
0.9448257350947955	0.7992777284036094	0.8289885395572867
0.2992777284036094	0.9448257350947955	0.5789885395572867
0.7007222715963906	0.0551742649052045	0.5789885395572867
0.9448257350947955	0.7007222715963906	0.4210114604427133
0.0551742649052045	0.2992777284036094	0.4210114604427133
0.2007222865963882	0.9448257350947955	0.1710114604427133
0.7992777284036094	0.0551742649052045	0.1710114604427133
0.5551742649052045	0.7007222715963906	0.3289885395572867
0.4448257350947955	0.2992777284036094	0.3289885395572867
0.4477575844049539	0.750000000000000	0.625000000000000
0.5522424155950461	0.250000000000000	0.625000000000000
0.750000000000000	0.5522424155950461	0.375000000000000
0.250000000000000	0.4477575844049539	0.375000000000000
0.0522424155950461	0.750000000000000	0.125000000000000
0.9477575844049539	0.250000000000000	0.125000000000000
0.250000000000000	0.0522424155950461	0.875000000000000
0.750000000000000	0.9477575844049539	0.875000000000000
0.250000000000000	0.9526906079036692	0.375000000000000
0.750000000000000	0.0473094000963314	0.375000000000000
0.9526906079036692	0.750000000000000	0.625000000000000
0.0473094000963314	0.250000000000000	0.625000000000000
0.5473093920963308	0.750000000000000	0.125000000000000
0.4526906079036692	0.250000000000000	0.125000000000000
0.750000000000000	0.4526906079036692	0.875000000000000
0.250000000000000	0.5473093920963308	0.875000000000000

8GPa

1.000000000000000		
8.0054732828689730	0.000000000000000	0.000000000000000
0.000000000000000	8.0054732828689730	0.000000000000000
0.000000000000000	0.000000000000000	5.6933214695340775

N	Zn	C
16	8	8

Direct

0.7976727774742685	0.4477899788248649	0.0788326687843295
0.2023272375257292	0.5522100211751351	0.0788326687843295
0.4477899788248649	0.2023272375257292	0.9211673312156705
0.5522100211751351	0.7976727774742685	0.9211673312156705
0.7023272225257315	0.4477899788248649	0.6711673312156705
0.2976727774742685	0.5522100211751351	0.6711673312156705
0.0522100211751351	0.2023272375257292	0.8288326687843295
0.9477899788248649	0.7976727774742685	0.8288326687843295
0.2976727774742685	0.9477899788248649	0.5788326687843295
0.7023272225257315	0.0522100211751351	0.5788326687843295
0.9477899788248649	0.7023272225257315	0.4211673312156705
0.0522100211751351	0.2976727774742685	0.4211673312156705
0.2023272375257292	0.9477899788248649	0.1711673312156705
0.7976727774742685	0.0522100211751351	0.1711673312156705
0.5522100211751351	0.7023272225257315	0.3288326687843295
0.4477899788248649	0.2976727774742685	0.3288326687843295
0.4461295498605367	0.750000000000000	0.625000000000000
0.5538704501394633	0.250000000000000	0.625000000000000
0.750000000000000	0.5538704501394633	0.375000000000000
0.250000000000000	0.4461295498605367	0.375000000000000
0.0538704501394633	0.750000000000000	0.125000000000000
0.9461295498605367	0.250000000000000	0.125000000000000
0.250000000000000	0.0538704501394633	0.875000000000000
0.750000000000000	0.9461295498605367	0.875000000000000
0.250000000000000	0.9562667232012956	0.375000000000000
0.750000000000000	0.0437332847987051	0.375000000000000
0.9562667232012956	0.750000000000000	0.625000000000000
0.0437332847987051	0.250000000000000	0.625000000000000
0.5437332767987044	0.750000000000000	0.125000000000000
0.4562667232012956	0.250000000000000	0.125000000000000
0.750000000000000	0.4562667232012956	0.875000000000000
0.250000000000000	0.5437332767987044	0.875000000000000

9GPa

1.000000000000000		
7.9200187047516604	0.000000000000000	0.000000000000000
0.000000000000000	7.9200187047518931	0.000000000000000
0.000000000000000	0.000000000000000	5.7184108375884213

N	Zn	C
16	8	8

Direct

0.7964991898297384	0.4504859632996343	0.0785182974129697
0.2035008251702592	0.5495140367003657	0.0785182974129697
0.4504859632996343	0.2035008251702592	0.9214817025870303
0.5495140367003657	0.7964991898297384	0.9214817025870303
0.7035008101702616	0.4504859632996343	0.6714817025870303
0.2964991898297384	0.5495140367003657	0.6714817025870303
0.0495140367003657	0.2035008251702592	0.8285182974129697
0.9504859632996343	0.7964991898297384	0.8285182974129697
0.2964991898297384	0.9504859632996343	0.5785182974129697
0.7035008101702616	0.0495140367003657	0.5785182974129697
0.9504859632996343	0.7035008101702616	0.4214817025870303
0.0495140367003657	0.2964991898297384	0.4214817025870303
0.2035008251702592	0.9504859632996343	0.1714817025870303
0.7964991898297384	0.0495140367003657	0.1714817025870303
0.5495140367003657	0.7035008101702616	0.3285182974129697
0.4504859632996343	0.2964991898297384	0.3285182974129697
0.4450739486278721	0.750000000000000	0.625000000000000
0.5549260513721279	0.250000000000000	0.625000000000000
0.750000000000000	0.5549260513721279	0.375000000000000
0.250000000000000	0.4450739486278721	0.375000000000000
0.0549260513721279	0.750000000000000	0.125000000000000
0.9450739486278721	0.250000000000000	0.125000000000000
0.250000000000000	0.0549260513721279	0.875000000000000
0.750000000000000	0.9450739486278721	0.875000000000000
0.250000000000000	0.9594691828256217	0.375000000000000
0.750000000000000	0.0405308251743790	0.375000000000000
0.9594691828256217	0.750000000000000	0.625000000000000
0.0405308251743790	0.250000000000000	0.625000000000000
0.5405308171743783	0.750000000000000	0.125000000000000
0.4594691828256217	0.250000000000000	0.125000000000000
0.750000000000000	0.4594691828256217	0.875000000000000
0.250000000000000	0.5405308171743783	0.875000000000000

10GPa

1.0000000000000000		
7.8363186457773448	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8363186457773528	0.0000000000000000
0.0000000000000000	0.0000000000000000	5.7409522463698828

N	Zn	C
16	8	8

Direct

0.7941352664414794	0.4536927847181431	0.0787301096543302
0.2058647485585183	0.5463072152818569	0.0787301096543302
0.4536927847181431	0.2058647485585183	0.9212698903456698
0.5463072152818569	0.7941352664414794	0.9212698903456698
0.7058647335585206	0.4536927847181431	0.6712698903456698
0.2941352664414794	0.5463072152818569	0.6712698903456698
0.0463072152818569	0.2058647485585183	0.8287301096543302
0.9536927847181431	0.7941352664414794	0.8287301096543302
0.2941352664414794	0.9536927847181431	0.5787301096543302
0.7058647335585206	0.0463072152818569	0.5787301096543302
0.9536927847181431	0.7058647335585206	0.4212698903456698
0.0463072152818569	0.2941352664414794	0.4212698903456698
0.2058647485585183	0.9536927847181431	0.1712698903456698
0.7941352664414794	0.0463072152818569	0.1712698903456698
0.5463072152818569	0.7058647335585206	0.3287301096543302
0.4536927847181431	0.2941352664414794	0.3287301096543302
0.4421068637869183	0.7500000000000000	0.6250000000000000
0.5578931362130817	0.2500000000000000	0.6250000000000000
0.7500000000000000	0.5578931362130817	0.3750000000000000
0.2500000000000000	0.4421068637869183	0.3750000000000000
0.0578931362130817	0.7500000000000000	0.1250000000000000
0.9421068637869183	0.2500000000000000	0.1250000000000000
0.2500000000000000	0.0578931362130817	0.8750000000000000
0.7500000000000000	0.9421068637869183	0.8750000000000000
0.2500000000000000	0.9634474382360096	0.3750000000000000
0.7500000000000000	0.0365525697639910	0.3750000000000000
0.9634474382360096	0.7500000000000000	0.6250000000000000
0.0365525697639910	0.2500000000000000	0.6250000000000000
0.5365525617639904	0.7500000000000000	0.1250000000000000
0.4634474382360096	0.2500000000000000	0.1250000000000000
0.7500000000000000	0.4634474382360096	0.8750000000000000
0.2500000000000000	0.5365525617639904	0.8750000000000000

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