Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Material

Tuning Conducting Phases in C3N/C2N Heterostructures: Applications in Thermoelectrics

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The phonon dispersion relation of the studied systems is shown in Figure S. 1.

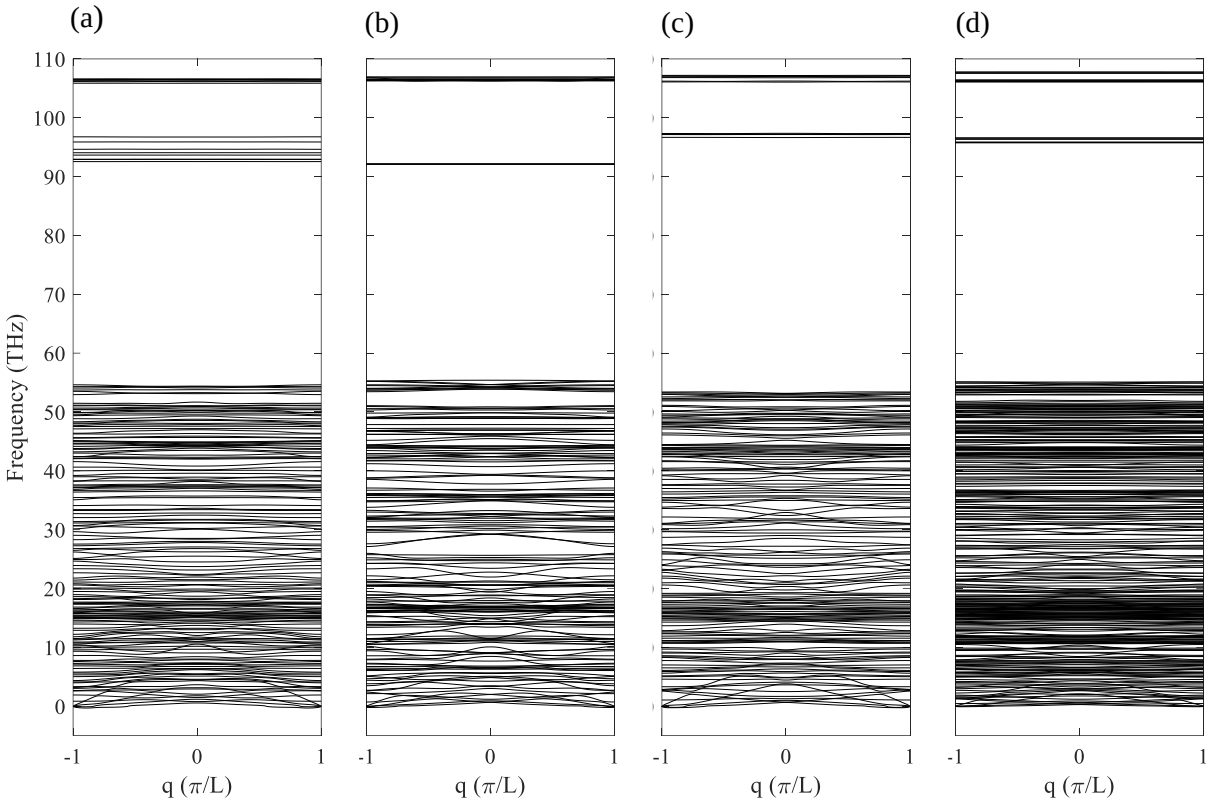

Figure S. 1. The phonon dispersion relation for the Model-A (a), Model-B (b), Model-C (c), and Model-D (d).

The temperature variation as a function of the time after the box relaxation and the NPT imposed ensemble at the pressure of zero and temperature of 300 K for the systems is presented in Figure S. 2.

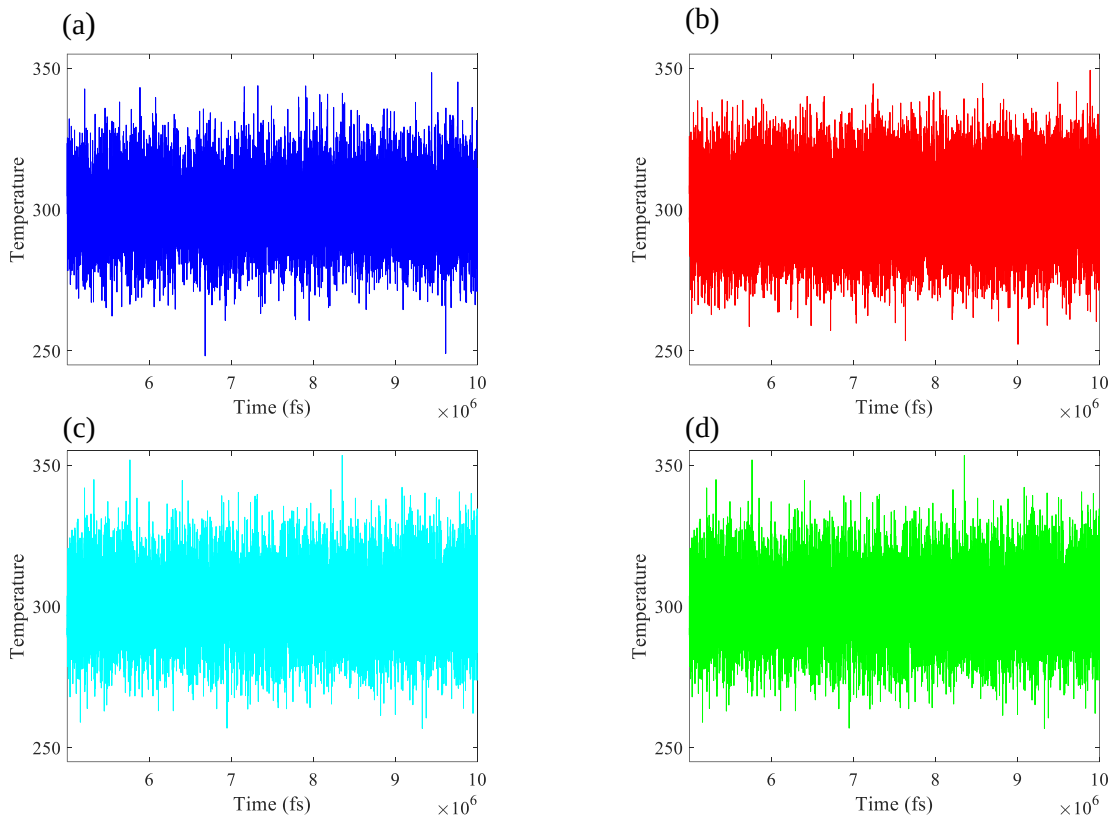

Figure S. 2. The variation of temperature vs. MD simulation time for the Model-A (a), Model-B (b), Model-C (c), and Model-D (d).

The phononic thermal conductivity as a function of temperature (Figure S. 3 (a)), and the zT as a function of chemical potential for the studied systems.

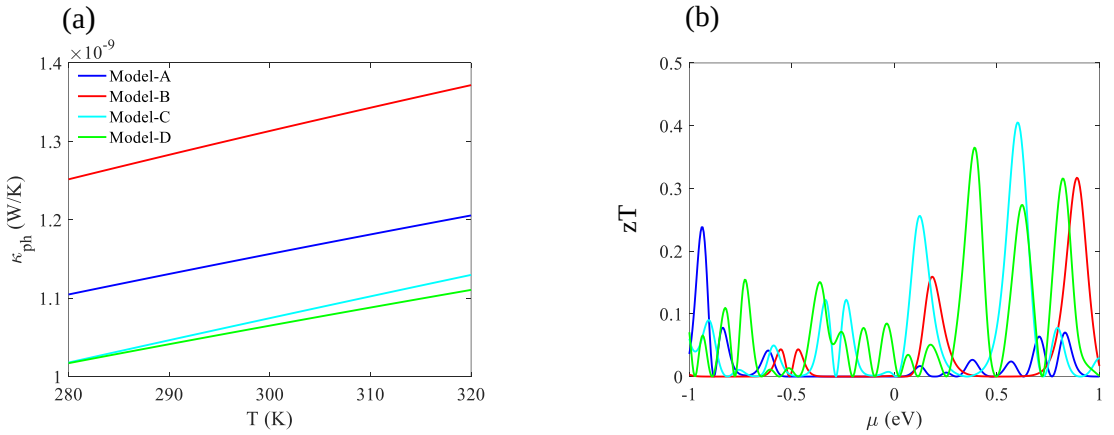

Figure S. 3. The phonon thermal conductivity as a function of temperature (a), and thermoelectric figure of merit as a function of chemical potential (b) for the Model-A (blue), Model-B (red), Model-C (cyan), and Model-D (green).

To have an insight about the corresponding carrier concentration (*n*) for the Model-D is plotted versus the chemical potential using the BotlzTrap2 code [1].

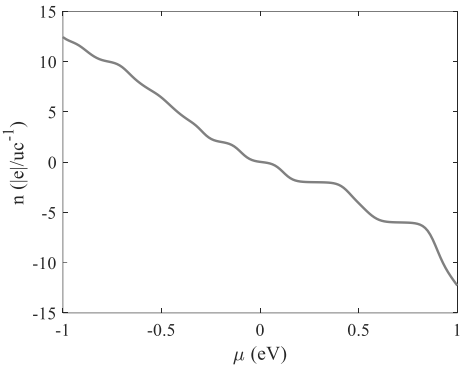

Figure S. 4. The carrier concentration as a function of the chemical potential for the Model-D at 300 K. The symbol uc represents unit cell volume.

The detailed results of the studied system are presented in the following figures.

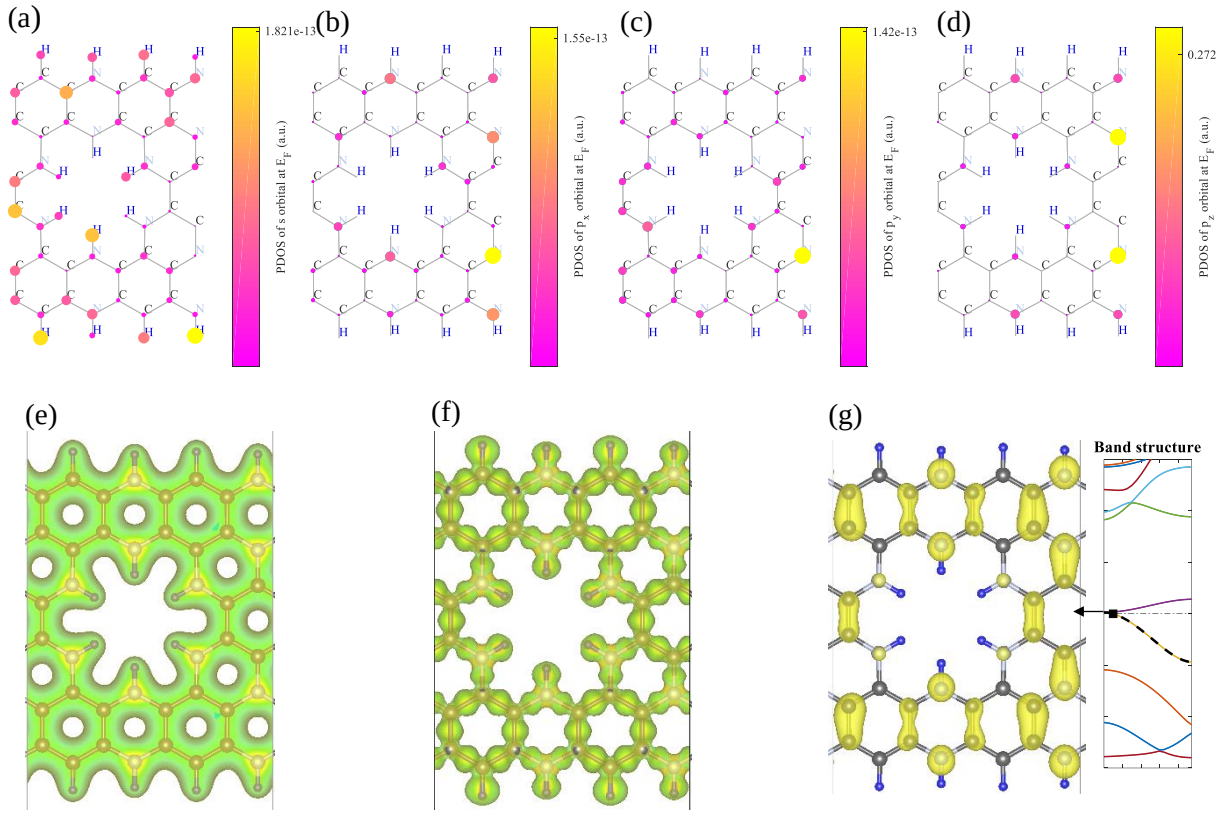

Figure S. 5. PDOS at E_F per orbital are shown in (a), (b), (c), and (d), respectively for s, p_x, p_y, and p_z. (e) The total charge density with isosurface value of 0.05 eV/Å^3, (f) ELF, and (g) wavefunction contribution at a specific k for a band marked by the filled square. The isosurface value for (f) and (g) is 0.001 eV/Å^3. All data are related to Model-B.

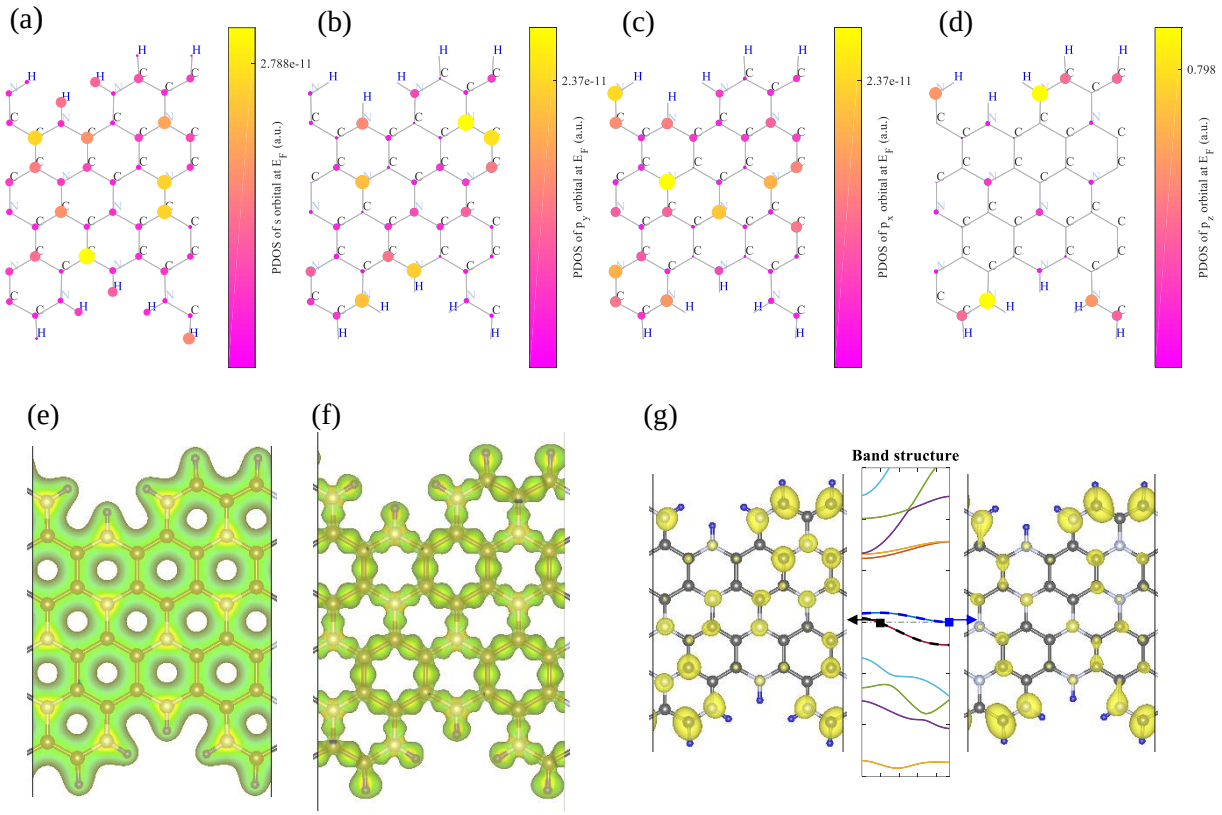

Figure S. 6. PDOS at E_F per orbital are shown in (a), (b), (c), and (d), respectively for s, p_x, p_y, and p_z. (e) The total charge density with isosurface value of 0.05 eV/Å^3, (f) ELF, and (g) wavefunction contribution at a specific k for a band marked by the filled square. The isosurface value for (f) and (g) is 0.001 eV/Å^3. All data are for Model-C.

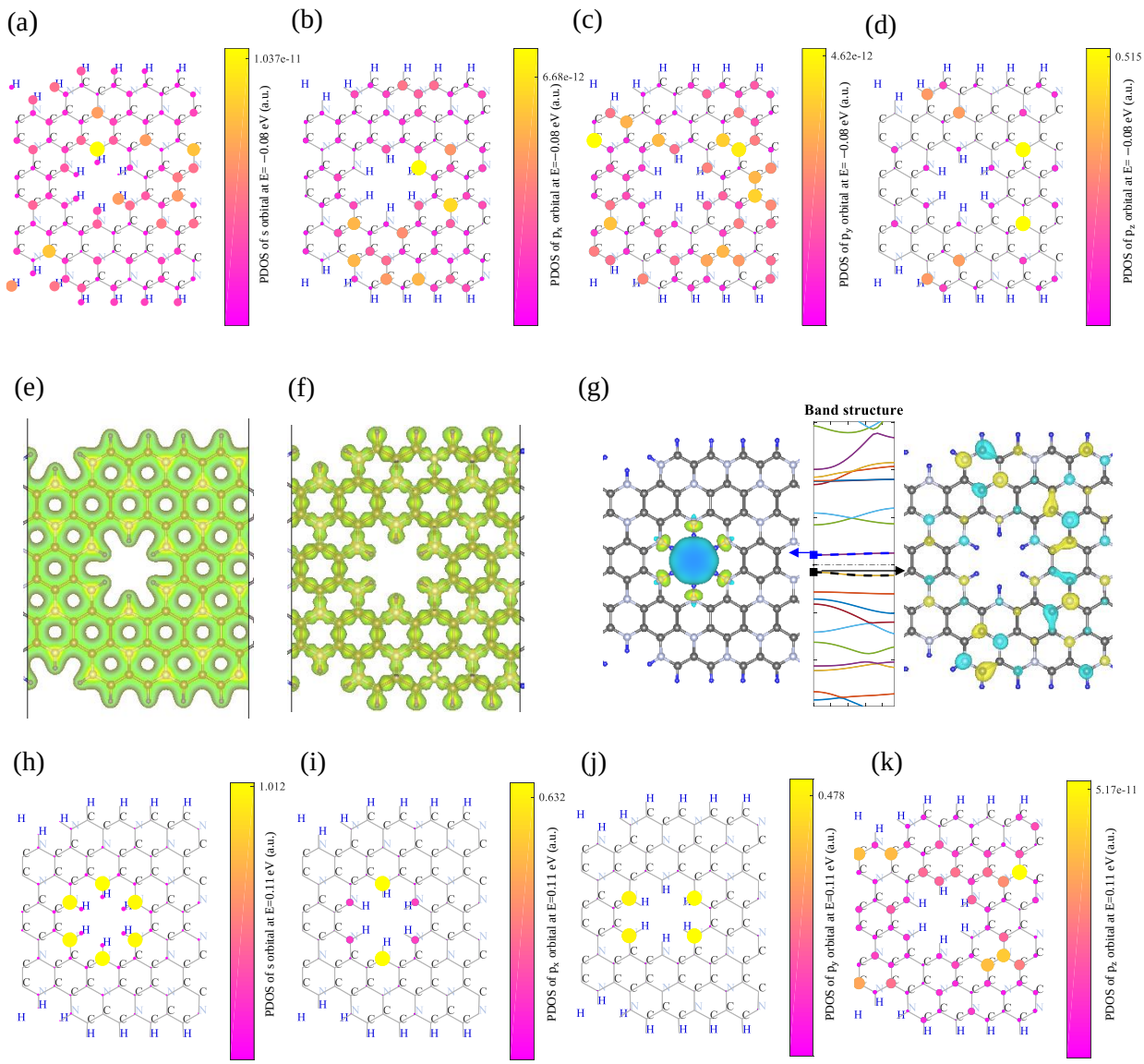

Figure S. 7. The orbital resolved PDOS map at E=−0.08 eV, corresponds to the first band below the Fermi energy are shown in (a), (b), (c), and (d), respectively for s, p_x, p_y, and p_z. (e) The total charge density with isosurface value of 0.05 eV/Å^3, (f) ELF, and (g) wavefunction contribution at a specific k for a specific band marked by the filled squares. The isosurface value for (f) and (g) is 0.001 eV/Å^3. The orbital resolved PDOS map at E=0.11 eV, corresponds to the first band above the Fermi energy are shown in (h), (i), (j), and (k), respectively for s, p_x, p_y, and p_z orbitals. All data are for Model-D.

The detailed results related to the convergence tests for Model-B and D are presented in the following tables. Since Model-A, B, and C unit cells are equal in dimension, and the number of atoms is close, just one system is checked and the results are used for the two other ones. We should note that we keep in mind to be careful about total stress value in the convergence test.

Table S. 1. The convergence test for Model-B. Selected values are shown in bold type.

Kinetic energy cutoff test (x periodic)						
ecutwfc	ecutrho	k-mesh	Total energy (Ry)	Dynamical RAM	Smearing	CPU-time
25	150	2×1×1	-906.02270387	2.51GB	0.01	1008.3
30	180	2×1×1	-907.38899093	3.30GB	0.01	1566.5
40	240	2×1×1	-907.83359292	5.05GB	0.01	3241.5
45	270	2×1×1	-907.85307082	6.03GB	0.01	4517.8
50	300	2×1×1	-907.85985770	7.10GB	0.01	5185.3
55	330	2×1×1	-907.86552173	8.18GB	0.01	5199.8
60	360	2×1×1	-907.87134923	9.33GB	0.01	7459.5
65	390	2×1×1	-907.87649208	10.47GB	0.01	7380.4
70	**420**	**2×1×1**	**-907.88026288**	**11.73GB**	**0.01**	**8852.0**
75	450	2×1×1	-907.88249786	12.97GB	0.01	8600.7
80	480	2×1×1	-907.88353995	14.28GB	0.01	10419.9
Charge density cutoff test						
70	210	2×1×1	-907.88001254	5.46GB	0.01	7092
70	**280**	**2×1×1**	**-907.88024723**	**7.27GB**	**0.01**	**6771.8**
70	350	2×1×1	-907.88023904	9.42GB	0.01	7769.2
k-mesh test						
70	280	3×1×1	-907.88357459	6.82GB	0.01	13546.3
70	280	4×1×1	-907.88500284	6.82GB	0.01	12618.4
70	280	5×1×1	-907.88513983	7.27GB	0.01	19422.5
70	**280**	**6×1×1**	**-907.88487113**	**7.27GB**	**0.01**	**18922.9**
70	280	7×1×1	-907.88485517	7.73GB	0.01	31061.3
Smearing test						
70	280	4×1×1	-907.88756243	6.82GB	0.02	12827
70	280	4×1×1	-907.88500284	6.82GB	0.01	12618.4
70	280	4×1×1	-907.8846152	6.82 GB	0.009	19857
70	280	4×1×1	-907.88422694	6.82GB	0.008	13865.9
70	**280**	**4×1×1**	**-907.88385047**	**6.82GB**	**0.007**	**12597.6**
70	280	4×1×1	-907.88349310	6.82GB	0.006	14893.6
70	280	4×1×1	-907.88315645	6.82GB	0.005	13680

Table S2. The convergence test for Model-D.

Kinetic energy cutoff test (x periodic)						
ecutwfc	ecutrho	k-mesh	Total Energy (Ry)	Dynamical Ram	Smearing	CPU-time
25	100	2×1×1	-1802.39557415	4.49GB	0.01	2992.3
30	120	2×1×1	-1804.96121632	5.90GB	0.01	4326.6
35	140	2×1×1	-1805.65516397	7.44GB	0.01	6113.5
40	160	2×1×1	-1805.83068765	9.08GB	0.01	8499

45	180	2×1×1	-1805.86724206	10.84GB	0.01	10110.9
50	200	2×1×1	-1805.87859099	12.68GB	0.01	14144.1
55	220	2×1×1	-1805.88924061	14.62GB	0.01	18251.1
60	240	2×1×1	-1805.90088082	14.62GB	0.01	18251.1
65	260	2×1×1	-1805.91130695	18.80GB	0.01	11756.2
70	280	2×1×1	-1805.91908903	21.00GB	0.01	18694
75	**300**	**2×1×1**	**-1805.92357049**	**23.33GB**	**0.01**	**26794**
80	320	2×1×1	-1805.92563949	25.67GB	0.01	31889
85	340	2×1×1	-1805.92643134	28.12GB	0.01	40050.1
90	360	2×1×1	-1805.92688751	30.69GB	0.01	52975
Charge density cutoff test						
75	150	2×1×1	-1805.92365712	18.62GB	0.01	20118.9
75	225	2×1×1	-1805.92310359	19.35GB	0.01	21627.4
75	**300**	**2×1×1**	**-1805.92357049**	**23.33GB**	**0.01**	**26794**
75	375	2×1×1	-1805.92354183	29.70GB	0.01	28190.2
k-mesh test						
75	**300**	**2×1×1**	**-1805.92357049**	**23.33GB**	**0.01**	**26794.0**
75	300	3×1×1	-1805.92276474	26.83GB	0.01	54415.2
75	300	4×1×1	-1805.92273003	26.83GB	0.01	50973.5
75	300	5×1×1	-1805.92273530	28.57GB	0.01	75606.4
Smearing test						
75	300	3×1×1	-1805.92093553	26.83GB	0.005	52707.2
75	300	3×1×1	-1805.92206133	26.83GB	0.0075	51370.2
75	300	3×1×1	-1805.92321905	26.83GB	0.0125	54181.9
75	300	2×1×1	-1805.92177262	23.33GB	0.005	26243.9
75	300	2×1×1	-1805.92286796	23.33GB	0.0075	26061.1
75	300	2×1×1	-1805.92357049	23.33GB	0.01	26794.0
75	300	2×1×1	-1805.92408161	23.33GB	0.0125	26673.2
75	300	2×1×1	-1805.92433255	23.33GB	0.015	26494.7
75	**300**	**2×1×1**	**-1805.92426690**	**23.33GB**	**0.0175**	**25757.3**
75	300	2×1×1	-1805.92394017	23.33GB	0.02	25076.7
75	300	2×1×1	-1805.92297171	23.33GB	0.025	24639.6
75	300	2×1×1	-1805.92209535	23.33GB	0.03	26715.5
75	300	2×1×1	-1805.92139671	23.33GB	0.035	26537.7
75	300	2×1×1	-1805.92073579	23.33GB	0.04	26454

The unit cell of the investigated models is presented in the following. The format of data is in crystal information file (cif).

Model-A:

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'global'
_cell_length_a                         9.655900
_cell_length_b                         27.000000
_cell_length_c                         15.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           3910.639501
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C          1.0     0.187357     0.293461     0.000000    Uiso  ? C
   C          1.0     0.687947     0.293461     0.000000    Uiso  ? C
   N          1.0     0.312053     0.370709     0.000000    Uiso  ? N
   C          1.0     0.187357     0.603547     0.000000    Uiso  ? C
   C          1.0     0.687936     0.603547     0.000000    Uiso  ? C
   C          1.0     0.938241     0.448502     0.000000    Uiso  ? C
   C          1.0     0.813534     0.525749     0.000000    Uiso  ? C
   C          1.0     0.563240     0.680790     0.000000    Uiso  ? C
   N          1.0     0.312053     0.680790     0.000000    Uiso  ? N
   N          1.0     0.812654     0.370709     0.000000    Uiso  ? N
   N          1.0     0.563240     0.319210     0.000000    Uiso  ? N
   C          1.0     0.312053     0.319210     0.000000    Uiso  ? C
   C          1.0     0.812643     0.319210     0.000000    Uiso  ? C
   N          1.0     0.812643     0.680790     0.000000    Uiso  ? N
   N          1.0     0.563240     0.629291     0.000000    Uiso  ? N
   C          1.0     0.312053     0.629291     0.000000    Uiso  ? C
   C          1.0     0.812643     0.629291     0.000000    Uiso  ? C
   N          1.0     0.813534     0.474251     0.000000    Uiso  ? N
   C          1.0     0.938230     0.551493     0.000000    Uiso  ? C
   C          1.0     0.687947     0.706539     0.000000    Uiso  ? C
   C          1.0     0.187357     0.706539     0.000000    Uiso  ? C
   C          1.0     0.187357     0.396458     0.000000    Uiso  ? C
   C          1.0     0.938241     0.396641     0.000000    Uiso  ? C
   C          1.0     0.938241     0.706722     0.000000    Uiso  ? C
```

```
   C          1.0     0.437641     0.706722     0.000000    Uiso  ? C
   C          1.0     0.187346     0.551682     0.000000    Uiso  ? C
   C          1.0     0.687947     0.551682     0.000000    Uiso  ? C
   C          1.0     0.938241     0.293278     0.000000    Uiso  ? C
   C          1.0     0.437641     0.293278     0.000000    Uiso  ? C
   C          1.0     0.938241     0.603359     0.000000    Uiso  ? C
   C          1.0     0.437652     0.603359     0.000000    Uiso  ? C
   C          1.0     0.187346     0.448318     0.000000    Uiso  ? C
   C          1.0     0.061759     0.474251     0.000000    Uiso  ? C
   N          1.0     0.062651     0.319210     0.000000    Uiso  ? N
   N          1.0     0.062651     0.629296     0.000000    Uiso  ? N
   N          1.0     0.061759     0.525749     0.000000    Uiso  ? N
   C          1.0     0.062651     0.680790     0.000000    Uiso  ? C
   C          1.0     0.062651     0.370709     0.000000    Uiso  ? C
   H          1.0     0.437638     0.253648     0.000000    Uiso  ? H
   H          1.0     0.938242     0.253648     0.000000    Uiso  ? H
   H          1.0     0.437638     0.746352     0.000000    Uiso  ? H
   H          1.0     0.938242     0.746352     0.000000    Uiso  ? H
   H          1.0     0.187357     0.746909     0.000000    Uiso  ? H
   H          1.0     0.687946     0.746909     0.000000    Uiso  ? H
   H          1.0     0.687946     0.253091     0.000000    Uiso  ? H
   H          1.0     0.187357     0.253091     0.000000    Uiso  ? H
   N          1.0     0.312053     0.474253     0.000000    Uiso  ? N
   N          1.0     0.563240     0.525747     0.000000    Uiso  ? N
   C          1.0     0.312053     0.525747     0.000000    Uiso  ? C
   C          1.0     0.437652     0.550766     0.000000    Uiso  ? C
   H          1.0     0.564941     0.486122     0.000000    Uiso  ? H
   H          1.0     0.408193     0.454545     0.000000    Uiso  ? H
   H          1.0     0.717567     0.454436     0.000000    Uiso  ? H
   H          1.0     0.563240     0.358840     0.000000    Uiso  ? H
   H          1.0     0.716691     0.390526     0.000000    Uiso  ? H
   H          1.0     0.408023     0.390522     0.000000    Uiso  ? H
```

Model-B :

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'global'
_cell_length_a                         9.655900
_cell_length_b                         27.000000
_cell_length_c                         15.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           3910.639501
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'
```

```
loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C          1.0     0.187357     0.293461     0.000000    Uiso  ? C
   C          1.0     0.687947     0.293461     0.000000    Uiso  ? C
   C          1.0     0.563240     0.370709     0.000000    Uiso  ? C
   C          1.0     0.312053     0.370709     0.000000    Uiso  ? C
   C          1.0     0.187357     0.603547     0.000000    Uiso  ? C
   C          1.0     0.687936     0.603547     0.000000    Uiso  ? C
   C          1.0     0.938241     0.448502     0.000000    Uiso  ? C
   C          1.0     0.813534     0.525749     0.000000    Uiso  ? C
   C          1.0     0.563240     0.680790     0.000000    Uiso  ? C
   C          1.0     0.312053     0.680790     0.000000    Uiso  ? C
   C          1.0     0.812654     0.370709     0.000000    Uiso  ? C
   C          1.0     0.563240     0.319210     0.000000    Uiso  ? C
   C          1.0     0.312053     0.319210     0.000000    Uiso  ? C
   C          1.0     0.812643     0.319210     0.000000    Uiso  ? C
   C          1.0     0.812643     0.680790     0.000000    Uiso  ? C
   C          1.0     0.563240     0.629291     0.000000    Uiso  ? C
   C          1.0     0.312053     0.629291     0.000000    Uiso  ? C
   C          1.0     0.812643     0.629291     0.000000    Uiso  ? C
   C          1.0     0.813534     0.474251     0.000000    Uiso  ? C
   C          1.0     0.938230     0.551493     0.000000    Uiso  ? C
   C          1.0     0.687947     0.706539     0.000000    Uiso  ? C
   C          1.0     0.187357     0.706539     0.000000    Uiso  ? C
   C          1.0     0.687947     0.396458     0.000000    Uiso  ? C
   C          1.0     0.187357     0.396458     0.000000    Uiso  ? C
   N          1.0     0.938241     0.396641     0.000000    Uiso  ? N
   N          1.0     0.437652     0.396641     0.000000    Uiso  ? N
   N          1.0     0.938241     0.706722     0.000000    Uiso  ? N
   N          1.0     0.437641     0.706722     0.000000    Uiso  ? N
   N          1.0     0.187346     0.551682     0.000000    Uiso  ? N
   N          1.0     0.687947     0.551682     0.000000    Uiso  ? N
   N          1.0     0.938241     0.293278     0.000000    Uiso  ? N
   N          1.0     0.437641     0.293278     0.000000    Uiso  ? N
   N          1.0     0.938241     0.603359     0.000000    Uiso  ? N
   N          1.0     0.437652     0.603359     0.000000    Uiso  ? N
   N          1.0     0.687947     0.448318     0.000000    Uiso  ? N
   N          1.0     0.187346     0.448318     0.000000    Uiso  ? N
   C          1.0     0.061759     0.474251     0.000000    Uiso  ? C
   C          1.0     0.062651     0.319210     0.000000    Uiso  ? C
   C          1.0     0.062651     0.629296     0.000000    Uiso  ? C
   C          1.0     0.061759     0.525749     0.000000    Uiso  ? C
   C          1.0     0.062651     0.680790     0.000000    Uiso  ? C
   C          1.0     0.062651     0.370709     0.000000    Uiso  ? C
   H          1.0     0.283315     0.468132     0.000000    Uiso  ? H
   H          1.0     0.591980     0.468133     0.000000    Uiso  ? H
```

```
   H          1.0     0.437653     0.563729     0.000000    Uiso  ? H
   H          1.0     0.437638     0.253648     0.000000    Uiso  ? H
   H          1.0     0.938242     0.253648     0.000000    Uiso  ? H
   H          1.0     0.591984     0.531864     0.000000    Uiso  ? H
   H          1.0     0.283315     0.531868     0.000000    Uiso  ? H
   H          1.0     0.437638     0.746352     0.000000    Uiso  ? H
   H          1.0     0.938242     0.746352     0.000000    Uiso  ? H
   H          1.0     0.437653     0.436271     0.000000    Uiso  ? H
   H          1.0     0.187357     0.746909     0.000000    Uiso  ? H
   H          1.0     0.687946     0.746909     0.000000    Uiso  ? H
   H          1.0     0.687946     0.253091     0.000000    Uiso  ? H
   H          1.0     0.187357     0.253091     0.000000    Uiso  ? H
```

Model-C:

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'global'
_cell_length_a                         9.655900
_cell_length_b                         27.000000
_cell_length_c                         15.000000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           3910.639501
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C          1.0     0.187357     0.293461     0.000000    Uiso  ? C
   N          1.0     0.563240     0.370709     0.000000    Uiso  ? N
   C          1.0     0.312053     0.370709     0.000000    Uiso  ? C
   C          1.0     0.187357     0.603547     0.000000    Uiso  ? C
   C          1.0     0.687936     0.603547     0.000000    Uiso  ? C
   C          1.0     0.938241     0.448502     0.000000    Uiso  ? C
   N          1.0     0.813534     0.525749     0.000000    Uiso  ? N
   N          1.0     0.563240     0.680790     0.000000    Uiso  ? N
   C          1.0     0.812654     0.370709     0.000000    Uiso  ? C
   N          1.0     0.312053     0.319210     0.000000    Uiso  ? N
   N          1.0     0.812643     0.319210     0.000000    Uiso  ? N
```

```
   C          1.0     0.812643     0.680790     0.000000    Uiso  ? C
   C          1.0     0.563240     0.629291     0.000000    Uiso  ? C
   N          1.0     0.312053     0.629291     0.000000    Uiso  ? N
   N          1.0     0.812643     0.629291     0.000000    Uiso  ? N
   C          1.0     0.813534     0.474251     0.000000    Uiso  ? C
   C          1.0     0.938230     0.551493     0.000000    Uiso  ? C
   C          1.0     0.687947     0.706539     0.000000    Uiso  ? C
   C          1.0     0.687947     0.396458     0.000000    Uiso  ? C
   C          1.0     0.187357     0.396458     0.000000    Uiso  ? C
   C          1.0     0.938241     0.396641     0.000000    Uiso  ? C
   C          1.0     0.437652     0.396641     0.000000    Uiso  ? C
   C          1.0     0.938241     0.706722     0.000000    Uiso  ? C
   C          1.0     0.187346     0.551682     0.000000    Uiso  ? C
   C          1.0     0.687947     0.551682     0.000000    Uiso  ? C
   C          1.0     0.938241     0.293278     0.000000    Uiso  ? C
   C          1.0     0.938241     0.603359     0.000000    Uiso  ? C
   C          1.0     0.437652     0.603359     0.000000    Uiso  ? C
   C          1.0     0.687947     0.448318     0.000000    Uiso  ? C
   C          1.0     0.187346     0.448318     0.000000    Uiso  ? C
   N          1.0     0.061759     0.474251     0.000000    Uiso  ? N
   C          1.0     0.062651     0.319210     0.000000    Uiso  ? C
   C          1.0     0.062651     0.629296     0.000000    Uiso  ? C
   C          1.0     0.061759     0.525749     0.000000    Uiso  ? C
   N          1.0     0.062651     0.680790     0.000000    Uiso  ? N
   N          1.0     0.062651     0.370709     0.000000    Uiso  ? N
   H          1.0     0.938242     0.253648     0.000000    Uiso  ? H
   H          1.0     0.938242     0.746352     0.000000    Uiso  ? H
   H          1.0     0.687946     0.746909     0.000000    Uiso  ? H
   H          1.0     0.187357     0.253091     0.000000    Uiso  ? H
   N          1.0     0.563240     0.474253     0.000000    Uiso  ? N
   C          1.0     0.312053     0.474253     0.000000    Uiso  ? C
   C          1.0     0.563240     0.525747     0.000000    Uiso  ? C
   N          1.0     0.312053     0.525747     0.000000    Uiso  ? N
   C          1.0     0.437652     0.550766     0.000000    Uiso  ? C
   C          1.0     0.437652     0.449234     0.000000    Uiso  ? C
   H          1.0     0.158617     0.700604     0.000000    Uiso  ? H
   H          1.0     0.312058     0.668921     0.000000    Uiso  ? H
   H          1.0     0.716676     0.299395     0.000000    Uiso  ? H
   H          1.0     0.408023     0.299397     0.000000    Uiso  ? H
   H          1.0     0.467273     0.700604     0.000000    Uiso  ? H
   H          1.0     0.563236     0.331079     0.000000    Uiso  ? H
```

Model-D:

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'global'
_cell_length_a                         14.478200
_cell_length_b                         32.000000
_cell_length_c                         15.000000
_cell_angle_alpha                      90.000000
```

```
_cell_angle_beta                        90.000000
_cell_angle_gamma                       90.000000
_cell_volume                            6949.535980
_space_group_name_H-M_alt               'P 1'
_space_group_IT_number                  1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   N          1.0     0.124955     0.587441     0.000000    Uiso  ? N
   N          1.0     0.791882     0.587441     0.000000    Uiso  ? N
   N          1.0     0.458811     0.587441     0.000000    Uiso  ? N
   C          1.0     0.375641     0.260016     0.000000    Uiso  ? C
   C          1.0     0.375641     0.652619     0.000000    Uiso  ? C
   C          1.0     0.208118     0.652619     0.000000    Uiso  ? C
   C          1.0     0.875045     0.260016     0.000000    Uiso  ? C
   C          1.0     0.875045     0.652619     0.000000    Uiso  ? C
   C          1.0     0.124955     0.456473     0.000000    Uiso  ? C
   C          1.0     0.791882     0.456473     0.000000    Uiso  ? C
   C          1.0     0.625740     0.325654     0.000000    Uiso  ? C
   N          1.0     0.625740     0.718257     0.000000    Uiso  ? N
   C          1.0     0.542569     0.390831     0.000000    Uiso  ? C
   C          1.0     0.208118     0.521647     0.000000    Uiso  ? C
   C          1.0     0.875045     0.521647     0.000000    Uiso  ? C
   C          1.0     0.541982     0.260016     0.000000    Uiso  ? C
   C          1.0     0.541982     0.652619     0.000000    Uiso  ? C
   C          1.0     0.375641     0.609167     0.000000    Uiso  ? C
   C          1.0     0.208118     0.609167     0.000000    Uiso  ? C
   C          1.0     0.875045     0.609167     0.000000    Uiso  ? C
   C          1.0     0.541975     0.609167     0.000000    Uiso  ? C
   C          1.0     0.208118     0.478195     0.000000    Uiso  ? C
   C          1.0     0.875045     0.478195     0.000000    Uiso  ? C
   C          1.0     0.542569     0.347379     0.000000    Uiso  ? C
   C          1.0     0.542569     0.739982     0.000000    Uiso  ? C
   C          1.0     0.625732     0.412553     0.000000    Uiso  ? C
   C          1.0     0.124955     0.543372     0.000000    Uiso  ? C
   C          1.0     0.791882     0.543372     0.000000    Uiso  ? C
   C          1.0     0.458811     0.281742     0.000000    Uiso  ? C
   N          1.0     0.458811     0.674344     0.000000    Uiso  ? N
   N          1.0     0.124955     0.674344     0.000000    Uiso  ? N
   C          1.0     0.791882     0.281742     0.000000    Uiso  ? C
   N          1.0     0.791882     0.674344     0.000000    Uiso  ? N
   N          1.0     0.625740     0.281896     0.000000    Uiso  ? N
   C          1.0     0.625740     0.674499     0.000000    Uiso  ? C
```

```
N          1.0     0.291883     0.281896     0.000000    Uiso  ? N
C          1.0     0.291883     0.674499     0.000000    Uiso  ? C
N          1.0     0.958810     0.281896     0.000000    Uiso  ? N
C          1.0     0.958810     0.674499     0.000000    Uiso  ? C
N          1.0     0.625740     0.543527     0.000000    Uiso  ? N
N          1.0     0.291876     0.543527     0.000000    Uiso  ? N
N          1.0     0.958803     0.543527     0.000000    Uiso  ? N
N          1.0     0.124948     0.412712     0.000000    Uiso  ? N
N          1.0     0.791875     0.412712     0.000000    Uiso  ? N
N          1.0     0.458811     0.412712     0.000000    Uiso  ? N
C          1.0     0.625740     0.587286     0.000000    Uiso  ? C
C          1.0     0.291876     0.587286     0.000000    Uiso  ? C
C          1.0     0.958803     0.587286     0.000000    Uiso  ? C
N          1.0     0.625740     0.456314     0.000000    Uiso  ? N
N          1.0     0.291883     0.456314     0.000000    Uiso  ? N
N          1.0     0.958810     0.456314     0.000000    Uiso  ? N
N          1.0     0.458811     0.325499     0.000000    Uiso  ? N
C          1.0     0.458811     0.718102     0.000000    Uiso  ? C
N          1.0     0.124948     0.325499     0.000000    Uiso  ? N
N          1.0     0.791875     0.325499     0.000000    Uiso  ? N
C          1.0     0.791875     0.718102     0.000000    Uiso  ? C
C          1.0     0.041190     0.347379     0.000000    Uiso  ? C
C          1.0     0.708117     0.347379     0.000000    Uiso  ? C
C          1.0     0.708117     0.739982     0.000000    Uiso  ? C
C          1.0     0.041785     0.609167     0.000000    Uiso  ? C
C          1.0     0.708712     0.609167     0.000000    Uiso  ? C
C          1.0     0.041785     0.478199     0.000000    Uiso  ? C
C          1.0     0.708712     0.478199     0.000000    Uiso  ? C
C          1.0     0.041190     0.390831     0.000000    Uiso  ? C
C          1.0     0.708117     0.390831     0.000000    Uiso  ? C
C          1.0     0.041785     0.521647     0.000000    Uiso  ? C
C          1.0     0.708712     0.521647     0.000000    Uiso  ? C
C          1.0     0.041785     0.652619     0.000000    Uiso  ? C
C          1.0     0.708712     0.260016     0.000000    Uiso  ? C
C          1.0     0.708712     0.652619     0.000000    Uiso  ? C
C          1.0     0.375641     0.347381     0.000000    Uiso  ? C
C          1.0     0.375641     0.739984     0.000000    Uiso  ? C
C          1.0     0.208118     0.347381     0.000000    Uiso  ? C
C          1.0     0.875045     0.347381     0.000000    Uiso  ? C
C          1.0     0.875045     0.739984     0.000000    Uiso  ? C
C          1.0     0.375641     0.390829     0.000000    Uiso  ? C
C          1.0     0.208118     0.390829     0.000000    Uiso  ? C
C          1.0     0.875045     0.390829     0.000000    Uiso  ? C
C          1.0     0.291883     0.411939     0.000000    Uiso  ? C
C          1.0     0.958810     0.411939     0.000000    Uiso  ? C
C          1.0     0.291883     0.326271     0.000000    Uiso  ? C
N          1.0     0.291883     0.718874     0.000000    Uiso  ? N
C          1.0     0.958810     0.326271     0.000000    Uiso  ? C
N          1.0     0.958810     0.718874     0.000000    Uiso  ? N
H          1.0     1.022240     0.736037     0.000000    Uiso  ? H
H          1.0     0.227880     0.735593     0.000000    Uiso  ? H
H          1.0     0.874810     0.774047     0.000000    Uiso  ? H
H          1.0     0.376797     0.774043     0.000000    Uiso  ? H
H          1.0     0.708401     0.225954     0.000000    Uiso  ? H
```

```
   H          1.0     0.707803     0.774045     0.000000    Uiso  ? H
   H          1.0     0.124945     0.292061     0.000000    Uiso  ? H
   H          1.0     0.355886     0.473033     0.000000    Uiso  ? H
   H          1.0     0.561740     0.473035     0.000000    Uiso  ? H
   H          1.0     0.458581     0.446149     0.000000    Uiso  ? H
   H          1.0     0.355880     0.526809     0.000000    Uiso  ? H
   H          1.0     0.561737     0.526809     0.000000    Uiso  ? H
   H          1.0     1.022810     0.265177     0.000000    Uiso  ? H
   H          1.0     0.227880     0.265178     0.000000    Uiso  ? H
   H          1.0     0.124955     0.707782     0.000000    Uiso  ? H
   H          1.0     0.542567     0.774045     0.000000    Uiso  ? H
   H          1.0     0.541982     0.225953     0.000000    Uiso  ? H
   H          1.0     0.875042     0.225953     0.000000    Uiso  ? H
   H          1.0     0.375639     0.225953     0.000000    Uiso  ? H
   H          1.0     0.458811     0.554004     0.000000    Uiso  ? H
```

Reference

[1] G. K. H. Madsen, J. Carrete, and M. J. Verstraete, *BoltzTraP2, a Program for Interpolating Band Structures and Calculating Semi-Classical Transport Coefficients*, Comput. Phys. Commun. **231**, 140 (2018).