# Supplemental Materials: Electronic and optical properties of sodium niobate: A density functional theory study

## I. SIMPLE CUBIC PEROVSKITE $Pm\bar{3}m$ PHASE

```
#=======================================
# CRYSTAL DATA
#---------------------
data_VESTA_phase_1
_chemical_name_common 'NaNbO3, Pm3m'
_cell_length_a 3.94422
_cell_length_b 3.94422
_cell_length_c 3.94422
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 90
_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_B_iso_or_equiv
_atom_site_type_symbol
Na1 1.0 0.500000 0.500000 0.500000 Biso 1.000000 Na
Nb1 1.0 0.000000 0.000000 0.000000 Biso 1.000000 Nb
O1 1.0 0.500000 0.000000 0.000000 Biso 1.000000 O
O2 1.0 0.000000 0.500000 0.000000 Biso 1.000000 O
O3 1.0 0.000000 0.000000 0.500000 Biso 1.000000 O
```

## II. RHOMBOHEDRAL *R3c* PHASE

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#=======================================
# CRYSTAL DATA
#---------------------
data_VESTA_phase_1
_chemical_name_common 'NaNbO3, R3c'
_cell_length_a 5.48921
_cell_length_b 5.48921
_cell_length_c 13.72048
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 120
_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_B_iso_or_equiv
_atom_site_type_symbol
Na1 1.0 0.000000 -0.000000 0.270769 Biso 1.000000 Na
Na2 1.0 0.000000 -0.000000 0.770769 Biso 1.000000 Na
Na3 1.0 0.666667 0.333333 0.604102 Biso 1.000000 Na
Na4 1.0 0.666667 0.333333 0.104102 Biso 1.000000 Na
Na5 1.0 0.333333 0.666667 0.937435 Biso 1.000000 Na
Na6 1.0 0.333333 0.666667 0.437435 Biso 1.000000 Na
Nb1 1.0 0.000000 -0.000000 0.012520 Biso 1.000000 Nb
Nb2 1.0 0.000000 -0.000000 0.512520 Biso 1.000000 Nb
Nb3 1.0 0.666667 0.333333 0.345853 Biso 1.000000 Nb
Nb4 1.0 0.666667 0.333333 0.845853 Biso 1.000000 Nb
Nb5 1.0 0.333333 0.666667 0.679186 Biso 1.000000 Nb
Nb6 1.0 0.333333 0.666667 0.179186 Biso 1.000000 Nb
O1 1.0 0.232419 0.895591 0.081737 Biso 1.000000 O
O2 1.0 0.104409 0.336828 0.081737 Biso 1.000000 O
O3 1.0 0.663172 0.767581 0.081737 Biso 1.000000 O
O4 1.0 0.104409 0.767581 0.581737 Biso 1.000000 O
O5 1.0 0.663172 0.895591 0.581737 Biso 1.000000 O
O6 1.0 0.232419 0.336828 0.581737 Biso 1.000000 O
O7 1.0 0.899086 0.228924 0.415071 Biso 1.000000 O
O8 1.0 0.771076 0.670162 0.415071 Biso 1.000000 O
O9 1.0 0.329838 0.100914 0.415071 Biso 1.000000 O
O10 1.0 0.771076 0.100914 0.915071 Biso 1.000000 O
O11 1.0 0.329838 0.228924 0.915071 Biso 1.000000 O
O12 1.0 0.899086 0.670162 0.915071 Biso 1.000000 O
O13 1.0 0.565752 0.562257 0.748404 Biso 1.000000 O
O14 1.0 0.437742 0.003495 0.748404 Biso 1.000000 O
O15 1.0 0.996505 0.434248 0.748404 Biso 1.000000 O
O16 1.0 0.437742 0.434248 0.248404 Biso 1.000000 O
O17 1.0 0.996505 0.562257 0.248404 Biso 1.000000 O
O18 1.0 0.565752 0.003495 0.248404 Biso 1.000000 O
```

## III. ORTHORHOMBIC *Pbcm* PHASE

```
#======================================
# CRYSTAL DATA
#--------------------------
data_VESTA_phase_1
_chemical_name_common 'NaNbO3, Pbcm'
_cell_length_a 5.49574
_cell_length_b 5.56164
_cell_length_c 15.49372
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 90
_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_B_iso_or_equiv
_atom_site_type_symbol
Na1 1.0 0.256517 0.250000 0.000000 Biso 1.000000 Na
Na2 1.0 0.743483 0.750000 0.000000 Biso 1.000000 Na
Na3 1.0 0.743483 0.750000 0.500000 Biso 1.000000 Na
Na4 1.0 0.256517 0.250000 0.500000 Biso 1.000000 Na
Na5 1.0 0.258164 0.209493 0.250000 Biso 1.000000 Na
Na6 1.0 0.741836 0.790507 0.750000 Biso 1.000000 Na
Na7 1.0 0.741836 0.709493 0.250000 Biso 1.000000 Na
Na8 1.0 0.258164 0.290507 0.750000 Biso 1.000000 Na
Nb1 1.0 0.245017 0.727863 0.125170 Biso 1.000000 Nb
Nb2 1.0 0.754983 0.272137 0.874830 Biso 1.000000 Nb
Nb3 1.0 0.754983 0.272137 0.625170 Biso 1.000000 Nb
Nb4 1.0 0.245017 0.727863 0.374830 Biso 1.000000 Nb
Nb5 1.0 0.754983 0.227863 0.374830 Biso 1.000000 Nb
Nb6 1.0 0.245017 0.772137 0.625170 Biso 1.000000 Nb
Nb7 1.0 0.245017 0.772137 0.874830 Biso 1.000000 Nb
Nb8 1.0 0.754983 0.227863 0.125170 Biso 1.000000 Nb
O1 1.0 0.687238 0.250000 0.000000 Biso 1.000000 O
O2 1.0 0.312762 0.750000 0.000000 Biso 1.000000 O
O3 1.0 0.312762 0.750000 0.500000 Biso 1.000000 O
O4 1.0 0.687238 0.250000 0.500000 Biso 1.000000 O
O5 1.0 0.186261 0.771647 0.250000 Biso 1.000000 O
O6 1.0 0.813739 0.228353 0.750000 Biso 1.000000 O
O7 1.0 0.813739 0.271647 0.250000 Biso 1.000000 O
O8 1.0 0.186261 0.728353 0.750000 Biso 1.000000 O
O9 1.0 0.462015 0.468063 0.141433 Biso 1.000000 O
O10 1.0 0.537985 0.531937 0.858567 Biso 1.000000 O
O11 1.0 0.537985 0.531937 0.641433 Biso 1.000000 O
O12 1.0 0.462015 0.468063 0.358567 Biso 1.000000 O
O13 1.0 0.537985 0.968063 0.358567 Biso 1.000000 O
O14 1.0 0.462015 0.031937 0.641433 Biso 1.000000 O
O15 1.0 0.462015 0.031937 0.858567 Biso 1.000000 O
O16 1.0 0.537985 0.968063 0.141433 Biso 1.000000 O
O17 1.0 0.039063 0.041511 0.109111 Biso 1.000000 O
O18 1.0 0.960937 0.958489 0.890889 Biso 1.000000 O
O19 1.0 0.960937 0.958489 0.609111 Biso 1.000000 O
O20 1.0 0.039063 0.041511 0.390889 Biso 1.000000 O
O21 1.0 0.960937 0.541511 0.390889 Biso 1.000000 O
O22 1.0 0.039063 0.458489 0.609111 Biso 1.000000 O
O23 1.0 0.039063 0.458489 0.890889 Biso 1.000000 O
O24 1.0 0.960937 0.541511 0.109111 Biso 1.000000 O
```

## IV. MONOCLINIC *Pm* PHASE

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#======================================
# CRYSTAL DATA
#--------------------------
data_VESTA_phase_1
_chemical_name_common 'NaNbO3, Pm'
_cell_length_a 5.49544
_cell_length_b 15.50413
_cell_length_c 5.55863
_cell_angle_alpha 90
_cell_angle_beta 90.06500
_cell_angle_gamma 90
_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_B_iso_or_equiv
_atom_site_type_symbol
Na1 1.0 0.293223 0.000000 0.825588 Biso 1.000000 Na
Na2 1.0 0.293390 0.500000 0.744631 Biso 1.000000 Na
Na3 1.0 0.291951 0.250080 0.785044 Biso 1.000000 Na
Na4 1.0 0.291951 0.749920 0.785044 Biso 1.000000 Na
Na5 1.0 0.777894 0.249950 0.285755 Biso 1.000000 Na
Na6 1.0 0.777894 0.750050 0.285755 Biso 1.000000 Na
Na7 1.0 0.776546 0.000000 0.325928 Biso 1.000000 Na
Na8 1.0 0.776778 0.500000 0.245057 Biso 1.000000 Na
Nb1 1.0 0.279678 0.124832 0.307158 Biso 1.000000 Nb
Nb2 1.0 0.279678 0.875168 0.307158 Biso 1.000000 Nb
Nb3 1.0 0.280050 0.624831 0.263225 Biso 1.000000 Nb
Nb4 1.0 0.280050 0.375169 0.263225 Biso 1.000000 Nb
Nb5 1.0 0.789836 0.124830 0.807314 Biso 1.000000 Nb
Nb6 1.0 0.789836 0.875170 0.807314 Biso 1.000000 Nb
Nb7 1.0 0.790195 0.624834 0.763390 Biso 1.000000 Nb
Nb8 1.0 0.790195 0.375166 0.763390 Biso 1.000000 Nb
O1 1.0 0.074799 0.140899 0.993108 Biso 1.000000 O
O2 1.0 0.074799 0.859101 0.993108 Biso 1.000000 O
O3 1.0 0.995078 0.640903 0.077404 Biso 1.000000 O
O4 1.0 0.995078 0.359097 0.077404 Biso 1.000000 O
O5 1.0 0.347005 0.250014 0.286075 Biso 1.000000 O
O6 1.0 0.347005 0.749986 0.286075 Biso 1.000000 O
O7 1.0 0.074336 0.640538 0.577337 Biso 1.000000 O
O8 1.0 0.074336 0.359462 0.577337 Biso 1.000000 O
O9 1.0 0.222082 0.000000 0.263019 Biso 1.000000 O
O10 1.0 0.847792 0.500000 0.807486 Biso 1.000000 O
O11 1.0 0.995531 0.140537 0.493167 Biso 1.000000 O
O12 1.0 0.995531 0.859463 0.493167 Biso 1.000000 O
O13 1.0 0.573653 0.108923 0.067672 Biso 1.000000 O
O14 1.0 0.573653 0.891077 0.067672 Biso 1.000000 O
O15 1.0 0.496206 0.608927 0.002821 Biso 1.000000 O
O16 1.0 0.496206 0.391073 0.002821 Biso 1.000000 O
O17 1.0 0.496777 0.108558 0.567489 Biso 1.000000 O
O18 1.0 0.496777 0.891442 0.567489 Biso 1.000000 O
O19 1.0 0.573103 0.608557 0.503013 Biso 1.000000 O
O20 1.0 0.573103 0.391443 0.503013 Biso 1.000000 O
O21 1.0 0.848280 0.000000 0.764343 Biso 1.000000 O
O22 1.0 0.221593 0.500000 0.306150 Biso 1.000000 O
O23 1.0 0.722868 0.249986 0.784377 Biso 1.000000 O
O24 1.0 0.722868 0.750014 0.784377 Biso 1.000000 O
```