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# Vacancy ordered structures in a nonstoichiometric niobium carbide $NbC_{0.83}$

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## Crystallographic data in CIF format

## Superstructure in Figure 1(*a*)

```
_chemical_name_common                  "
_cell_length_a                         5.51762
_cell_length_b                         9.56610
_cell_length_c                         10.99761
_cell_angle_alpha                      90
_cell_angle_beta                       109.43247
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'C 2'
_space_group_IT_number                 5

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, y, -z'
   'x+1/2, y+1/2, z'
   '-x+1/2, y+1/2, -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
   Nb1     1.0     0.261908     0.176402     0.125877     Uiso  0.050000 Nb
   Nb2     1.0     0.230854     0.500000     0.126957     Uiso  0.050000 Nb
   Nb3     1.0     0.265328     0.823047     0.133300     Uiso  0.050000 Nb
   Nb4     1.0     0.234673     0.010289     0.366702     Uiso  0.050000 Nb
   Nb5     1.0     0.269146     0.334024     0.373045     Uiso  0.050000 Nb
   Nb6     1.0     0.238094     0.656935     0.374125     Uiso  0.050000 Nb
   C1      1.0     0.000000     0.333775     0.000000     Uiso  0.050000 C
   C2      1.0     0.000000     0.664820     0.000000     Uiso  0.050000 C
   C3      1.0     0.000000     0.000000     0.500000     Uiso  0.050000 C
   C4      1.0     0.000000     0.664801     0.500000     Uiso  0.050000 C
   C5      1.0     0.000000     0.166669     0.250001     Uiso  0.050000 C
   C6      1.0    -0.000472     0.499593     0.250230     Uiso  0.050000 C
   C7      1.0     0.000276     0.833660     0.249813     Uiso  0.050000 C
```

## Superstructure in Figure 1(*b)*

```
_chemical_name_common                  "
_cell_length_a                         5.52137
_cell_length_b                         9.54661
_cell_length_c                         5.50524
_cell_angle_alpha                      90
_cell_angle_beta                       109.73413
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'C 2/m'
_space_group_IT_number                 12

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, y, -z'
   'x, -y, z'
   'x+1/2, y+1/2, z'
   '-x+1/2, -y+1/2, -z'
   '-x+1/2, y+1/2, -z'
   'x+1/2, -y+1/2, 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
   Nb1     1.0     0.264829      0.000000      0.735692     Uiso  0.050000 Nb
   Nb2     1.0     0.240752      0.676565      0.746371     Uiso  0.050000 Nb
   C1      1.0     0.000000      0.500000      0.500000     Uiso  0.050000 C
   C2      1.0     0.000000      0.333300      0.000000     Uiso  0.050000 C
   C3      1.0     0.000000      0.166700      0.500000     Uiso  0.050000 C
```

## Superstructure in Figure 2(*a)*

```
_chemical_name_common                  "
_cell_length_a                       7.09616
_cell_length_b                       7.78228
_cell_length_c                       5.50385
_cell_angle_alpha                   89.70044
_cell_angle_beta                    75.59914
_cell_angle_gamma                  111.16089
_space_group_name_H-M_alt             'P -1'
_space_group_IT_number                 2

loop_
_space_group_symop_operation_xyz
  'x, y, z'
  '-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
  Nb1        1.0     0.138698     0.046576     0.181715    Biso  1.000000 Nb
  Nb2        1.0     0.132493     0.703361     0.543729    Biso  1.000000 Nb
  Nb3        1.0     0.122512     0.380622     0.895048    Biso  1.000000 Nb
  Nb4        1.0     0.617595     0.880618     0.372762    Biso  1.000000 Nb
  Nb5        1.0     0.607646     0.526906     0.718429    Biso  1.000000 Nb
  Nb6        1.0     0.373081     0.791461     0.958862    Biso  1.000000 Nb
  C1         1.0    0.122617     0.877205     0.872310    Biso  1.000000 C
  C2         1.0    0.875587     0.459438     0.789163    Biso  1.000000 C
  C3         1.0    0.625891     0.374634     0.376609    Biso  1.000000 C
  C4         1.0    0.626938     0.041312     0.705643    Biso  1.000000 C
  C5         1.0    0.373068     0.290600     0.959473    Biso  1.000000 C
```

## Superstructure in Figure 2(*b)*

```
_chemical_name_common                  "
_cell_length_a                         10.00395
_cell_length_b                         4.51230
_cell_length_c                         6.33649
_cell_angle_alpha                      90
_cell_angle_beta                       108.85002
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'C 2/m'
_space_group_IT_number                 12

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, y, -z'
   'x, -y, z'
   'x+1/2, y+1/2, z'
   '-x+1/2, -y+1/2, -z'
   '-x+1/2, y+1/2, -z'
   'x+1/2, -y+1/2, 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
   Nb1        1.0     0.169538      0.000000      0.338829     Biso  1.000000 Nb
   Nb2        1.0     0.824813      0.000000      0.169310     Biso  1.000000 Nb
   Nb3        1.0     0.000000      0.500000      0.000000     Biso  1.000000 Nb
   Nb4        1.0     0.000000      0.500000      0.500000     Biso  1.000000 Nb
   C1         1.0     0.665707      0.000000      0.835065     Biso  1.000000 C
   C2         1.0     0.331784      0.000000      0.665432     Biso  1.000000 C
   C3         1.0     0.000000      0.000000      0.500000     Biso  1.000000 C
```

## Superstructure in Figure 2(*c*)

```
_chemical_name_common                  "
_cell_length_a                         13.40484
_cell_length_b                         4.51742
_cell_length_c                         9.97439
_cell_angle_alpha                      90
_cell_angle_beta                       116.48864
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'C 2/m'
_space_group_IT_number                 12

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, y, -z'
   'x, -y, z'
   'x+1/2, y+1/2, z'
   '-x+1/2, -y+1/2, -z'
   '-x+1/2, y+1/2, -z'
   'x+1/2, -y+1/2, 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
   Nb1        1.0     0.209831     0.000000     0.372167    Biso  1.000000 Nb
   Nb2        1.0     0.037106     0.000000     0.874821    Biso  1.000000 Nb
   Nb3        1.0     0.539937     0.000000     0.372951    Biso  1.000000 Nb
   Nb4        1.0     0.620395     0.000000     0.123146    Biso  1.000000 Nb
   Nb5        1.0     0.291609     0.000000     0.124547    Biso  1.000000 Nb
   Nb6        1.0     0.123852     0.000000     0.617870    Biso  1.000000 Nb
   C1         1.0     0.291526     0.000000     0.625327    Biso  1.000000 C
   C2         1.0     0.458118     0.000000     0.124949    Biso  1.000000 C
   C3         1.0     0.042217     0.000000     0.376880    Biso  1.000000 C
   C4         1.0     0.124945     0.000000     0.123446    Biso  1.000000 C
   C5         1.0     0.372968     0.000000     0.368099    Biso  1.000000 C
```

## Superstructure in Figure 2(*d*)

```
_chemical_name_common                  "
_cell_length_a                         4.48435
_cell_length_b                         13.33794
_cell_length_c                         4.50072
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'C m m m'
_space_group_IT_number                 65

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x, -y, z'
   'x, y, -z'
   '-x, y, -z'
   'x, -y, z'
   'x, -y, -z'
   '-x, y, z'
   'x+1/2, y+1/2, z'
   '-x+1/2, -y+1/2, -z'
   '-x+1/2, -y+1/2, z'
   'x+1/2, y+1/2, -z'
   '-x+1/2, y+1/2, -z'
   'x+1/2, -y+1/2, z'
   'x+1/2, -y+1/2, -z'
   '-x+1/2, y+1/2, 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
   Nb1        1.0     0.000000      0.329543      0.500000     Biso  1.000000 Nb
   Nb2        1.0     0.000000      0.163087      0.000000     Biso  1.000000 Nb
   Nb3        1.0     0.500000      0.000000      0.000000     Biso  1.000000 Nb
   Nb4        1.0     0.000000      0.000000      0.500000     Biso  1.000000 Nb
   C1         1.0     0.000000      0.334611      0.000000     Biso  1.000000 C
   C2         1.0     0.000000      0.167390      0.500000     Biso  1.000000 C
   C3         1.0     0.000000      0.000000      0.000000     Biso  1.000000 C
```

## Superstructure with space group $P3_1$

```
_chemical_name_common                  "
_cell_length_a                         5.47473
_cell_length_b                         5.47473
_cell_length_c                         15.45053
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_space_group_name_H-M_alt              'P 31'
_space_group_IT_number                 144

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-y, x-y, z+1/3'
   '-x+y, -x, z+2/3'

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
   C1         1.0    0.444079     0.555955     0.166448     Biso  1.000000 C
   C2         1.0    0.774786     0.225262     0.166447     Biso  1.000000 C
   C3         1.0    0.112426     0.556215     0.333125     Biso  1.000000 C
   C4         1.0    0.433066     0.216536     0.333117     Biso  1.000000 C
   C5         1.0    0.789687     0.894846     0.333111     Biso  1.000000 C
   Nb1        1.0    0.112121     0.551136     0.081872     Biso  1.000000 Nb
   Nb2        1.0    0.449503     0.226644     0.082088     Biso  1.000000 Nb
   Nb3        1.0    0.773588     0.889253     0.082036     Biso  1.000000 Nb
   Nb4        1.0    0.112091     0.560981     0.584385     Biso  1.000000 Nb
   Nb5        1.0    0.449464     0.222835     0.584162     Biso  1.000000 Nb
   Nb6        1.0    0.773566     0.884325     0.584208     Biso  1.000000 Nb
```