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Electronic Supplementary Information for

Elucidating the structure of the graphitic carbon nitride nanomaterials using X-ray photoelectron spectroscopy and X-ray powder diffraction techniques

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[b.] *Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France.*
[c.] **E-mail: mariop@amu.edu.pl*

The structure models used for the refinement of gCN

1. gCN P21212_500C

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  C2    1.0  0.655200  0.528000  0.250000  Uiso  0.012700 C
  C3    1.0  0.221600  0.798000  0.250000  Uiso  0.012700 C
  C4    1.0  0.778400  0.202000  0.250000  Uiso  0.012700 C
  C5    1.0  0.269500  0.630000  0.250000  Uiso  0.012700 C
  C6    1.0  0.730500  0.370000  0.250000  Uiso  0.012700 C
  C7    1.0  0.136100  0.648000  0.250000  Uiso  0.012700 C
  C8    1.0  0.864000  0.352000  0.250000  Uiso  0.012700 C
  C9    1.0  0.987200  0.683000  0.250000  Uiso  0.012700 C
  C10   1.0  0.012800  0.317000  0.250000  Uiso  0.012700 C
  C11   1.0  0.072900  0.820000  0.250000  Uiso  0.012700 C
  C12   1.0  0.927100  0.180000  0.250000  Uiso  0.012700 C
  C13   1.0  0.834400  0.028000  0.250000  Uiso  0.012700 C
  C14   1.0  0.165600  0.972000  0.250000  Uiso  0.012700 C
  C15   1.0  0.711200  0.702000  0.250000  Uiso  0.012700 C
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C16	1.0	0.288800	0.298000	0.250000	Uiso	0.012700 C
C17	1.0	0.759100	0.870000	0.250000	Uiso	0.012700 C
C18	1.0	0.240900	0.130000	0.250000	Uiso	0.012700 C
C19	1.0	0.625700	0.852000	0.250000	Uiso	0.012700 C
C20	1.0	0.374300	0.148000	0.250000	Uiso	0.012700 C
C21	1.0	0.478000	0.817000	0.250000	Uiso	0.012700 C
C22	1.0	0.522000	0.183000	0.250000	Uiso	0.012700 C
C23	1.0	0.562500	0.680000	0.250000	Uiso	0.012700 C
C24	1.0	0.437500	0.320000	0.250000	Uiso	0.012700 C
H1	1.0	0.874900	0.889100	0.250000	Uiso	0.012700 H
H2	1.0	0.125100	0.110900	0.250000	Uiso	0.012700 H
H3	1.0	0.385300	0.610900	0.250000	Uiso	0.012700 H
H4	1.0	0.614700	0.389100	0.250000	Uiso	0.012700 H
H5	1.0	0.916500	0.557600	0.250000	Uiso	0.012700 H
H6	1.0	0.083500	0.442400	0.250000	Uiso	0.012700 H
H7	1.0	0.407300	0.942400	0.250000	Uiso	0.012700 H
H8	1.0	0.592700	0.057600	0.250000	Uiso	0.012700 H
H9	1.0	0.358300	0.821700	0.250000	Uiso	0.012700 H
H10	1.0	0.641700	0.178300	0.250000	Uiso	0.012700 H
H11	1.0	0.867400	0.678300	0.250000	Uiso	0.012700 H
H12	1.0	0.132600	0.321700	0.250000	Uiso	0.012700 H
N1	1.0	0.142200	0.762000	0.250000	Uiso	0.012700 N
N2	1.0	0.857800	0.238000	0.250000	Uiso	0.012700 N
N3	1.0	0.088200	0.935000	0.250000	Uiso	0.012700 N
N4	1.0	0.911800	0.065000	0.250000	Uiso	0.012700 N
N5	1.0	0.226700	0.904000	0.250000	Uiso	0.012700 N
N6	1.0	0.773300	0.096000	0.250000	Uiso	0.012700 N
N7	1.0	0.282700	0.733000	0.250000	Uiso	0.012700 N
N8	1.0	0.717300	0.267000	0.250000	Uiso	0.012700 N
N9	1.0	0.198200	0.588000	0.250000	Uiso	0.012700 N

N10	1.0	0.801800	0.412000	0.250000	Uiso	0.012700 N
N11	1.0	0.057600	0.608000	0.250000	Uiso	0.012700 N
N12	1.0	0.942300	0.392000	0.250000	Uiso	0.012700 N
N13	1.0	0.997300	0.788000	0.250000	Uiso	0.012700 N
N14	1.0	0.002700	0.212000	0.250000	Uiso	0.012700 N
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N17	1.0	0.921000	0.638000	0.250000	Uiso	0.012700 N
N18	1.0	0.079000	0.362000	0.250000	Uiso	0.012700 N
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N20	1.0	0.368200	0.262000	0.250000	Uiso	0.012700 N
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N24	1.0	0.283700	0.404000	0.250000	Uiso	0.012700 N
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N26	1.0	0.227700	0.233000	0.250000	Uiso	0.012700 N
N27	1.0	0.687800	0.912000	0.250000	Uiso	0.012700 N
N28	1.0	0.312200	0.088000	0.250000	Uiso	0.012700 N
N29	1.0	0.547300	0.892000	0.250000	Uiso	0.012700 N
N30	1.0	0.452700	0.108000	0.250000	Uiso	0.012700 N
N31	1.0	0.488200	0.712000	0.250000	Uiso	0.012700 N
N32	1.0	0.511800	0.288000	0.250000	Uiso	0.012700 N
N33	1.0	0.823200	0.932000	0.250000	Uiso	0.012700 N
N34	1.0	0.176800	0.068000	0.250000	Uiso	0.012700 N
N35	1.0	0.411800	0.862000	0.250000	Uiso	0.012700 N
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2. gCN P21212_550C

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C3	1.0	0.221600	0.798000	0.250000	Uiso	0.012700 C
C4	1.0	0.778400	0.202000	0.250000	Uiso	0.012700 C
C5	1.0	0.269500	0.630000	0.250000	Uiso	0.012700 C
C6	1.0	0.730500	0.370000	0.250000	Uiso	0.012700 C
C7	1.0	0.136100	0.648000	0.250000	Uiso	0.012700 C
C8	1.0	0.864000	0.352000	0.250000	Uiso	0.012700 C
C9	1.0	0.987200	0.683000	0.250000	Uiso	0.012700 C
C10	1.0	0.012800	0.317000	0.250000	Uiso	0.012700 C
C11	1.0	0.072900	0.820000	0.250000	Uiso	0.012700 C
C12	1.0	0.927100	0.180000	0.250000	Uiso	0.012700 C
C13	1.0	0.834400	0.028000	0.250000	Uiso	0.012700 C
C14	1.0	0.165600	0.972000	0.250000	Uiso	0.012700 C
C15	1.0	0.711200	0.702000	0.250000	Uiso	0.012700 C
C16	1.0	0.288800	0.298000	0.250000	Uiso	0.012700 C
C17	1.0	0.759100	0.870000	0.250000	Uiso	0.012700 C
C18	1.0	0.240900	0.130000	0.250000	Uiso	0.012700 C
C19	1.0	0.625700	0.852000	0.250000	Uiso	0.012700 C
C20	1.0	0.374300	0.148000	0.250000	Uiso	0.012700 C
C21	1.0	0.478000	0.817000	0.250000	Uiso	0.012700 C
C22	1.0	0.522000	0.183000	0.250000	Uiso	0.012700 C
C23	1.0	0.562500	0.680000	0.250000	Uiso	0.012700 C
C24	1.0	0.437500	0.320000	0.250000	Uiso	0.012700 C
H1	1.0	0.874900	0.889100	0.250000	Uiso	0.012700 H
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H3	1.0	0.385300	0.610900	0.250000	Uiso	0.012700 H
H4	1.0	0.614700	0.389100	0.250000	Uiso	0.012700 H

H5	1.0	0.916500	0.557600	0.250000	Uiso	0.012700 H
H6	1.0	0.083500	0.442400	0.250000	Uiso	0.012700 H
H7	1.0	0.407300	0.942400	0.250000	Uiso	0.012700 H
H8	1.0	0.592700	0.057600	0.250000	Uiso	0.012700 H
H9	1.0	0.358300	0.821700	0.250000	Uiso	0.012700 H
H10	1.0	0.641700	0.178300	0.250000	Uiso	0.012700 H
H11	1.0	0.867400	0.678300	0.250000	Uiso	0.012700 H
H12	1.0	0.132600	0.321700	0.250000	Uiso	0.012700 H
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N2	1.0	0.857800	0.238000	0.250000	Uiso	0.012700 N
N3	1.0	0.088200	0.935000	0.250000	Uiso	0.012700 N
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N7	1.0	0.282700	0.733000	0.250000	Uiso	0.012700 N
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N15	1.0	0.333600	0.568000	0.250000	Uiso	0.012700 N
N16	1.0	0.666400	0.432000	0.250000	Uiso	0.012700 N
N17	1.0	0.921000	0.638000	0.250000	Uiso	0.012700 N
N18	1.0	0.079000	0.362000	0.250000	Uiso	0.012700 N
N19	1.0	0.631800	0.738000	0.250000	Uiso	0.012700 N
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N21	1.0	0.577800	0.565000	0.250000	Uiso	0.012700 N
N22	1.0	0.422200	0.435000	0.250000	Uiso	0.012700 N

N23	1.0	0.716300	0.596000	0.250000	Uiso	0.012700 N
N24	1.0	0.283700	0.404000	0.250000	Uiso	0.012700 N
N25	1.0	0.772300	0.767000	0.250000	Uiso	0.012700 N
N26	1.0	0.227700	0.233000	0.250000	Uiso	0.012700 N
N27	1.0	0.687800	0.912000	0.250000	Uiso	0.012700 N
N28	1.0	0.312200	0.088000	0.250000	Uiso	0.012700 N
N29	1.0	0.547300	0.892000	0.250000	Uiso	0.012700 N
N30	1.0	0.452700	0.108000	0.250000	Uiso	0.012700 N
N31	1.0	0.488200	0.712000	0.250000	Uiso	0.012700 N
N32	1.0	0.511800	0.288000	0.250000	Uiso	0.012700 N
N33	1.0	0.823200	0.932000	0.250000	Uiso	0.012700 N
N34	1.0	0.176800	0.068000	0.250000	Uiso	0.012700 N
N35	1.0	0.411800	0.862000	0.250000	Uiso	0.012700 N
N36	1.0	0.588200	0.138000	0.250000	Uiso	0.012700 N

3. gCN P21212_600C

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# CRYSTAL DATA

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_cell_length_b                         12.30900
_cell_length_c                         6.43790
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 21 21 2'
_space_group_IT_number                 18

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  'x+1/2, -y+1/2, -z'

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C1	1.0	0.344800	0.472000	0.250000	Uiso	0.012700 C
C2	1.0	0.655200	0.528000	0.250000	Uiso	0.012700 C
C3	1.0	0.221600	0.798000	0.250000	Uiso	0.012700 C
C4	1.0	0.778400	0.202000	0.250000	Uiso	0.012700 C
C5	1.0	0.269500	0.630000	0.250000	Uiso	0.012700 C
C6	1.0	0.730500	0.370000	0.250000	Uiso	0.012700 C
C7	1.0	0.136100	0.648000	0.250000	Uiso	0.012700 C
C8	1.0	0.864000	0.352000	0.250000	Uiso	0.012700 C
C9	1.0	0.987200	0.683000	0.250000	Uiso	0.012700 C
C10	1.0	0.012800	0.317000	0.250000	Uiso	0.012700 C
C11	1.0	0.072900	0.820000	0.250000	Uiso	0.012700 C
C12	1.0	0.927100	0.180000	0.250000	Uiso	0.012700 C
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C14	1.0	0.165600	0.972000	0.250000	Uiso	0.012700 C
C15	1.0	0.711200	0.702000	0.250000	Uiso	0.012700 C
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C17	1.0	0.759100	0.870000	0.250000	Uiso	0.012700 C
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C21	1.0	0.478000	0.817000	0.250000	Uiso	0.012700 C
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C23	1.0	0.562500	0.680000	0.250000	Uiso	0.012700 C
C24	1.0	0.437500	0.320000	0.250000	Uiso	0.012700 C
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H2	1.0	0.125100	0.110900	0.250000	Uiso	0.012700 H
H3	1.0	0.385300	0.610900	0.250000	Uiso	0.012700 H
H4	1.0	0.614700	0.389100	0.250000	Uiso	0.012700 H

H5	1.0	0.916500	0.557600	0.250000	Uiso	0.012700 H
H6	1.0	0.083500	0.442400	0.250000	Uiso	0.012700 H
H7	1.0	0.407300	0.942400	0.250000	Uiso	0.012700 H
H8	1.0	0.592700	0.057600	0.250000	Uiso	0.012700 H
H9	1.0	0.358300	0.821700	0.250000	Uiso	0.012700 H
H10	1.0	0.641700	0.178300	0.250000	Uiso	0.012700 H
H11	1.0	0.867400	0.678300	0.250000	Uiso	0.012700 H
H12	1.0	0.132600	0.321700	0.250000	Uiso	0.012700 H
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N2	1.0	0.857800	0.238000	0.250000	Uiso	0.012700 N
N3	1.0	0.088200	0.935000	0.250000	Uiso	0.012700 N
N4	1.0	0.911800	0.065000	0.250000	Uiso	0.012700 N
N5	1.0	0.226700	0.904000	0.250000	Uiso	0.012700 N
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N7	1.0	0.282700	0.733000	0.250000	Uiso	0.012700 N
N8	1.0	0.717300	0.267000	0.250000	Uiso	0.012700 N
N9	1.0	0.198200	0.588000	0.250000	Uiso	0.012700 N
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N15	1.0	0.333600	0.568000	0.250000	Uiso	0.012700 N
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N19	1.0	0.631800	0.738000	0.250000	Uiso	0.012700 N
N20	1.0	0.368200	0.262000	0.250000	Uiso	0.012700 N
N21	1.0	0.577800	0.565000	0.250000	Uiso	0.012700 N
N22	1.0	0.422200	0.435000	0.250000	Uiso	0.012700 N

N23	1.0	0.716300	0.596000	0.250000	Uiso	0.012700 N
N24	1.0	0.283700	0.404000	0.250000	Uiso	0.012700 N
N25	1.0	0.772300	0.767000	0.250000	Uiso	0.012700 N
N26	1.0	0.227700	0.233000	0.250000	Uiso	0.012700 N
N27	1.0	0.687800	0.912000	0.250000	Uiso	0.012700 N
N28	1.0	0.312200	0.088000	0.250000	Uiso	0.012700 N
N29	1.0	0.547300	0.892000	0.250000	Uiso	0.012700 N
N30	1.0	0.452700	0.108000	0.250000	Uiso	0.012700 N
N31	1.0	0.488200	0.712000	0.250000	Uiso	0.012700 N
N32	1.0	0.511800	0.288000	0.250000	Uiso	0.012700 N
N33	1.0	0.823200	0.932000	0.250000	Uiso	0.012700 N
N34	1.0	0.176800	0.068000	0.250000	Uiso	0.012700 N
N35	1.0	0.411800	0.862000	0.250000	Uiso	0.012700 N
N36	1.0	0.588200	0.138000	0.250000	Uiso	0.012700 N

4. gCN P-6m2_500

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_gC3N4 P-6m2_500


_chemical_name_common                  ''
_cell_length_a                         7.96700
_cell_length_b                         7.96700
_cell_length_c                         6.5117
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_space_group_name_H-M_alt              'P -6 m 2'
_space_group_IT_number                 187

loop_
_space_group_symop_operation_xyz
  'x, y, z'
  '-y, x-y, z'
  '-x+y, -x, z'
  'x, y, -z'
  '-y, x-y, -z'
  '-x+y, -x, -z'
  '-y, -x, z'
  '-x+y, y, z'
  'x, x-y, z'
  '-y, -x, -z'
  '-x+y, y, -z'
  'x, 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

N1	1.0	0.000000	0.000000	0.000000	Uiso	0.012700	N
N7	1.0	0.666667	0.666667	0.000000	Uiso	1.000000	N
N5	1.0	0.666667	0.333333	0.000000	Uiso	1.000000	N
N10	1.0	0.333333	0.333333	0.500000	Uiso	0.012700	N
N13	1.0	0.333333	0.666667	0.500000	Uiso	0.012700	N
N11	1.0	0.666667	0.333333	0.500000	Uiso	0.012700	N
N9	1.0	0.333333	0.333333	0.000000	Uiso	0.012700	N
N12	1.0	0.666667	0.666667	0.500000	Uiso	0.012700	N
C1	1.0	0.222200	0.111100	0.000000	Uiso	0.012700	C
C2	1.0	0.555500	0.111100	0.000000	Uiso	0.012700	C
C7	1.0	0.222200	0.444400	0.500000	Uiso	0.012700	C
C8	1.0	0.555500	0.444400	0.500000	Uiso	0.012700	C

5. gCN P-6m2_550

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_gC3N4 P-6m2_550



_chemical_name_common                  ''
_cell_length_a                         7.93800
_cell_length_b                         7.93800
_cell_length_c                         6.4725
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_space_group_name_H-M_alt              'P -6 m 2'
_space_group_IT_number                 187

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

'x, 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

N1	1.0	0.000000	0.000000	0.000000	Uiso	0.012700 N
N7	1.0	0.666667	0.666667	0.000000	Uiso	1.000000 N
N5	1.0	0.666667	0.333333	0.000000	Uiso	1.000000 N
N10	1.0	0.333333	0.333333	0.500000	Uiso	0.012700 N
N13	1.0	0.333333	0.666667	0.500000	Uiso	0.012700 N
N11	1.0	0.666667	0.333333	0.500000	Uiso	0.012700 N
N9	1.0	0.333333	0.333333	0.000000	Uiso	0.012700 N
N12	1.0	0.666667	0.666667	0.500000	Uiso	0.012700 N
C1	1.0	0.222200	0.111100	0.000000	Uiso	0.012700 C
C2	1.0	0.555500	0.111100	0.000000	Uiso	0.012700 C
C7	1.0	0.222200	0.444400	0.500000	Uiso	0.012700 C
C8	1.0	0.555500	0.444400	0.500000	Uiso	0.012700 C

6. gCN P-6m2_600

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_gC3N4 P-6m2_600


_chemical_name_common                  ''
_cell_length_a                         7.94600
_cell_length_b                         7.94600
_cell_length_c                         6.4420
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_space_group_name_H-M_alt              'P -6 m 2'
_space_group_IT_number                 187

loop_
_space_group_symop_operation_xyz
  'x, y, z'
  '-y, x-y, z'
  '-x+y, -x, z'
  'x, y, -z'
  '-y, x-y, -z'
  '-x+y, -x, -z'
  '-y, -x, z'
  '-x+y, y, z'
  'x, x-y, z'
  '-y, -x, -z'
  '-x+y, y, -z'
  'x, 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
  N1       1.0    0.000000     0.000000     0.000000    Uiso  0.012700 N
  N7       1.0    0.666667     0.666667     0.000000    Uiso  1.000000 N
  N5       1.0    0.666667     0.333333     0.000000    Uiso  1.000000 N
  N10      1.0    0.333333     0.333333     0.500000    Uiso  0.012700 N
  N13      1.0    0.333333     0.666667     0.500000    Uiso  0.012700 N
  N11      1.0    0.666667     0.333333     0.500000    Uiso  0.012700 N
  N9       1.0    0.333333     0.333333     0.000000    Uiso  0.012700 N
  N12      1.0    0.666667     0.666667     0.500000    Uiso  0.012700 N
  C1       1.0    0.222200     0.111100     0.000000    Uiso  0.012700 C
  C2       1.0    0.555500     0.111100     0.000000    Uiso  0.012700 C
  C7       1.0    0.222200     0.444400     0.500000    Uiso  0.012700 C
  C8       1.0    0.555500     0.444400     0.500000    Uiso  0.012700 C
```