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Supporting information for

"Superhard carbon nitride with metal-free magnetism assembled from two-dimensional C4N3: a first-principles study"

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Table S1. The crystallographic information of the six systems, including crystal parameters, fractional atomic coordinates, is listed below.

Cm-I: a=b=4.9897,c=10.2518, $\alpha = \beta =$ 134.5624,$\gamma = 60.8673$

Atom	x	y	z
C1	0.40436	-0.11212	-0.09017
C	0.21669	-0.29753	-0.44160
C	-0.95201	-0.45803	-0.76102
N	-0.67650	-0.19484	-0.00673
N	-0.81837	-0.36319	-0.33677
N	-0.05081	-0.54721	-0.68973
C	0.29144	-0.70857	-0.02436
C	0.40318	-0.59682	-0.08410
C	0.14304	-0.85696	-0.34441
N	-0.41773	-0.41773	-0.42291
N	-0.53539	-0.53539	-0.64420
C	-0.76039	-0.76039	-0.41971
C	-0.02247	-0.02247	-0.66973
C	-0.95104	-0.95104	-0.76607
N	-0.19029	-0.19029	-0.00565

Cm-II: a=b=4.9043,c=4.0476, $\alpha = \beta =$ 93.7759,$\gamma = 62.6579$

Atom	x	y	z
C	0.54333	0.02835	0.95329
C	0.35048	-0.13620	0.41687
N	0.40357	-0.14680	0.06849
N	0.48988	-0.96154	0.58845
C	0.36535	-0.63465	0.08524
C	0.54204	-0.45796	0.94933

C	0.52697	-0.47303	0.57018
C	0.35142	-0.64858	0.46577
N	0.89116	-0.10884	0.04569
N	-0.00446	-0.00446	0.41649

Cm-III: a=b=4.8130,c= 4.2925, $\alpha = \beta =$ 88.7375,$\gamma =$ 63.0970

Atom	x	y	z
C	0.05112	0.53499	0.92309
C	0.80494	-0.71636	0.59235
N	0.23686	0.70919	0.90777
N	0.99869	-0.54437	0.60557
C	0.72092	-0.27908	0.04461
C	0.53707	-0.46293	0.06583
N	0.98553	-0.01447	0.44753
C	0.48470	0.48470	0.41528
C	0.29322	0.29322	0.43312
N	0.23982	0.23982	0.11010

P1: a=4.99,b= 4.95,c= 5.03, $\alpha = 113.10,\beta = 80.30,\gamma = 120.33$

Atom	x	y	Z
C	0.552	0.514	-0.163
C	-0.084	-0.257	-0.126
C	0.392	0.136	-0.334
C	0.384	0.678	-0.239
N	0.087	0.049	-0.193
N	0.086	-0.439	-0.201
N	0.558	-0.054	-0.344

C2/m: a=b= 4.9400,c= 4.1623, $\alpha = \beta = 83.9437,\gamma = 60.7075$

Atom	x	y	z
C	-0.17628	-0.66072	0.18101
N	-0.35723	-0.83299	0.18872
C	-0.85129	0.14871	0.30154
C	-0.67203	0.32797	0.34018
N	-0.35876	-0.35876	0.31376

P-6m2:a= b=5.0060,c= 4.0499, , $\alpha = \beta = 90,\gamma = 120$

Atom	x	y	z
C	0.66667	0.33333	0.18848
C	0.01503	0.50751	0.30629
N	0.17237	0.34474	0.18618

Table S2: The corresponding mechanical stability criteria for the triclinic, Monoclinic, and hexagonal crystal systems.

For triclinic system (P1):

$C11>0$,

$C11C22-C12^2>0$

$$\begin{vmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{vmatrix} > 0, \quad \begin{vmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{12} & C_{22} & C_{23} & C_{24} \\ C_{13} & C_{23} & C_{33} & C_{34} \\ C_{14} & C_{24} & C_{34} & C_{44} \end{vmatrix} > 0, \quad \begin{vmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} \end{vmatrix} > 0, \quad \begin{vmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{vmatrix} > 0$$

For monoclinic systems (Cm and C2/m):

$C11>0$, $C22>0$, $C33>0$, $C44>0$, $C55>0$, $C66>0$,

$[C11+ C22+ C33+2(C12+C13+ C23)]>0$,

$(C33C55-C_{35}^2)>0$,$(C44C66-C_{46}^2)>0$,$(C22+C33-2C23)>0$,

$[C22(C33C55-C_{35}^2)+2C23C25C35-C_{23}^2C55-C_{25}^2C33]>0$,

$\{2[C15C25(C33C12-C13C23)+C15C35(C22C13-C12C23)+C25C35(C11C23-C12C13)]-[C_{15}^2(C22C33-C_{23}^2)+C_{25}^2(C11C33-C_{13}^2)+C_{35}^2(C11C22-C_{12}^2)]+C55g\}>0$

$g=C11C22C33-C11C_{23}^2-C22C_{13}^2-C33C_{12}^2+2C12C13C23$,

For the hexagonal system (P-6m2):

$C11>|C12|$, $C44>0$, $2C_{13}^2<C33(C11+C12)$

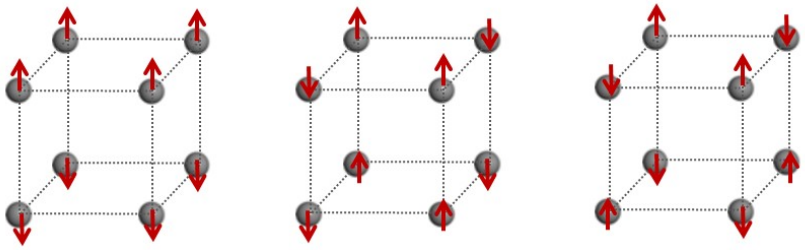

Fig. S1. The diagram of three types of anti-ferromagnetic configurations (A-type, C-type, and G-type) considered in this work.