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Two Isomeric Solid Carbon Nitrides with 1:1 Stoichiometry which Reveal Strong Mechanical Anisotropy

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SUPPORTING INFORMATION

New J. Chem

LIST OF SUPPLEMENTARY FIGURES AND TABLES:

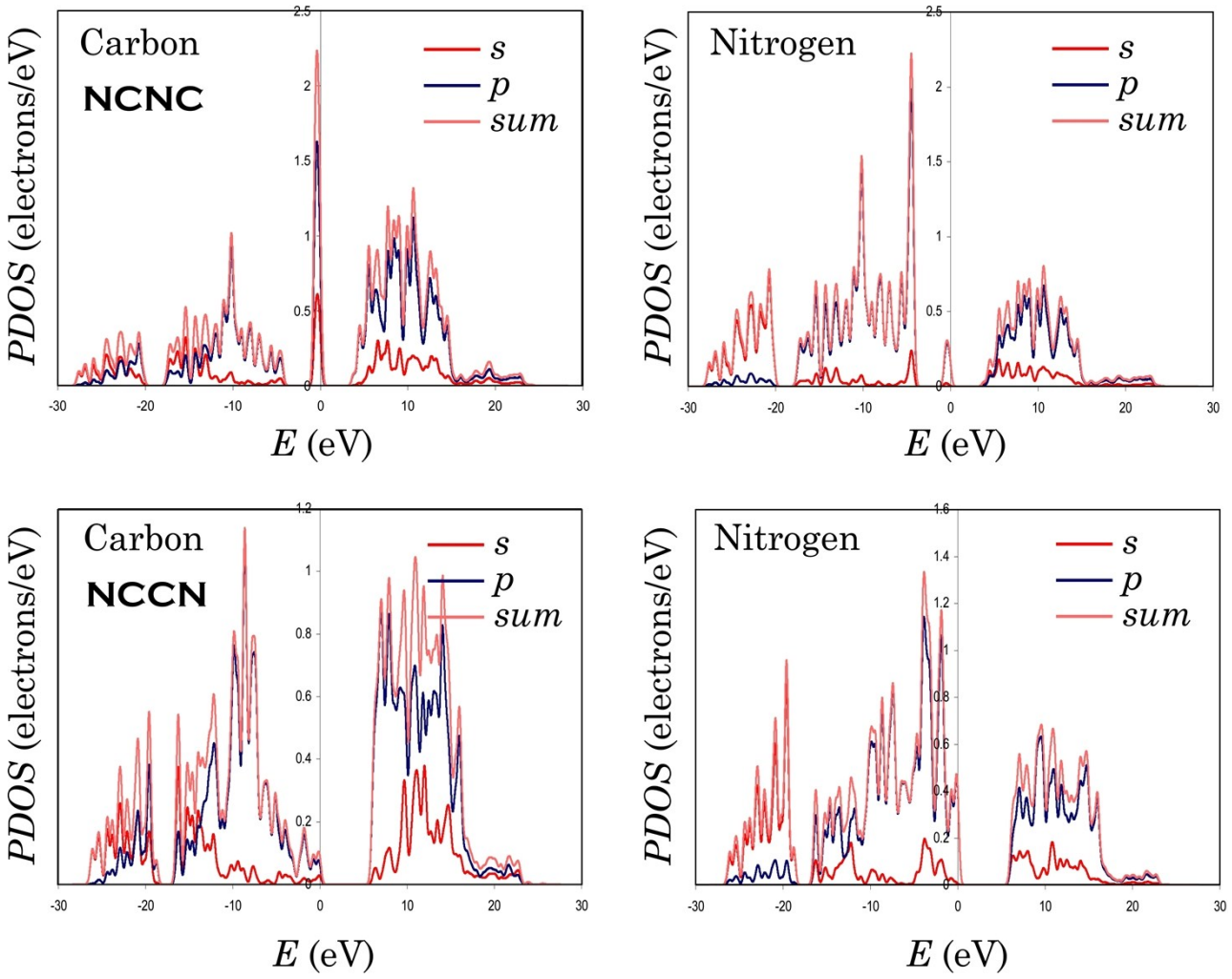

Fig. S1. Partial density of states of **NCNC** and **NCCN**.

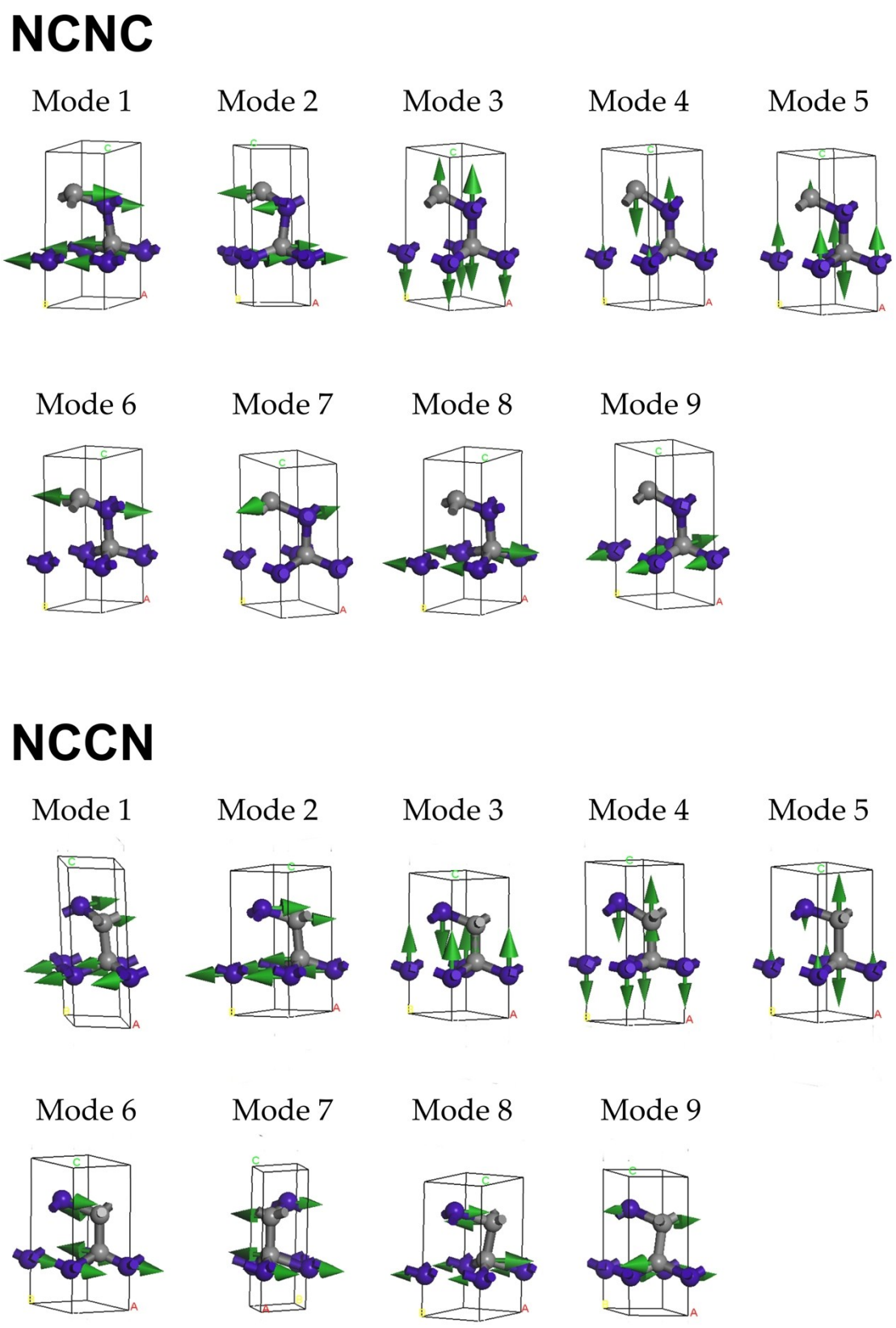

Fig. S2. Graphical description of the vibrational modes in the calculated spectrum of the **NCNC** and **NCCN** crystals.

Reflectivity

$$R(\omega)=\left|\frac{\sqrt{\varepsilon(\omega)}-1}{\sqrt{\varepsilon(\omega)}+1}\right|^2 \qquad \text{(S1)}$$

Refractive Index

$$n(\omega)=\frac{\sqrt{2}}{2}\left[\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}+\varepsilon_1(\omega)\right]^{1/2} \qquad \text{(S2)}$$

Conductivity

$$\sigma(\omega)=\sigma_1(\omega)+i\sigma_2(\omega)=-i\frac{\omega}{4\pi}\left(\varepsilon(\omega)-1\right) \qquad \text{(S3)}$$

Loss Function

$$\beta(\omega)=\mathrm{Im}\left(\frac{-1}{\varepsilon(\omega)}\right) \qquad \text{(S4)}$$

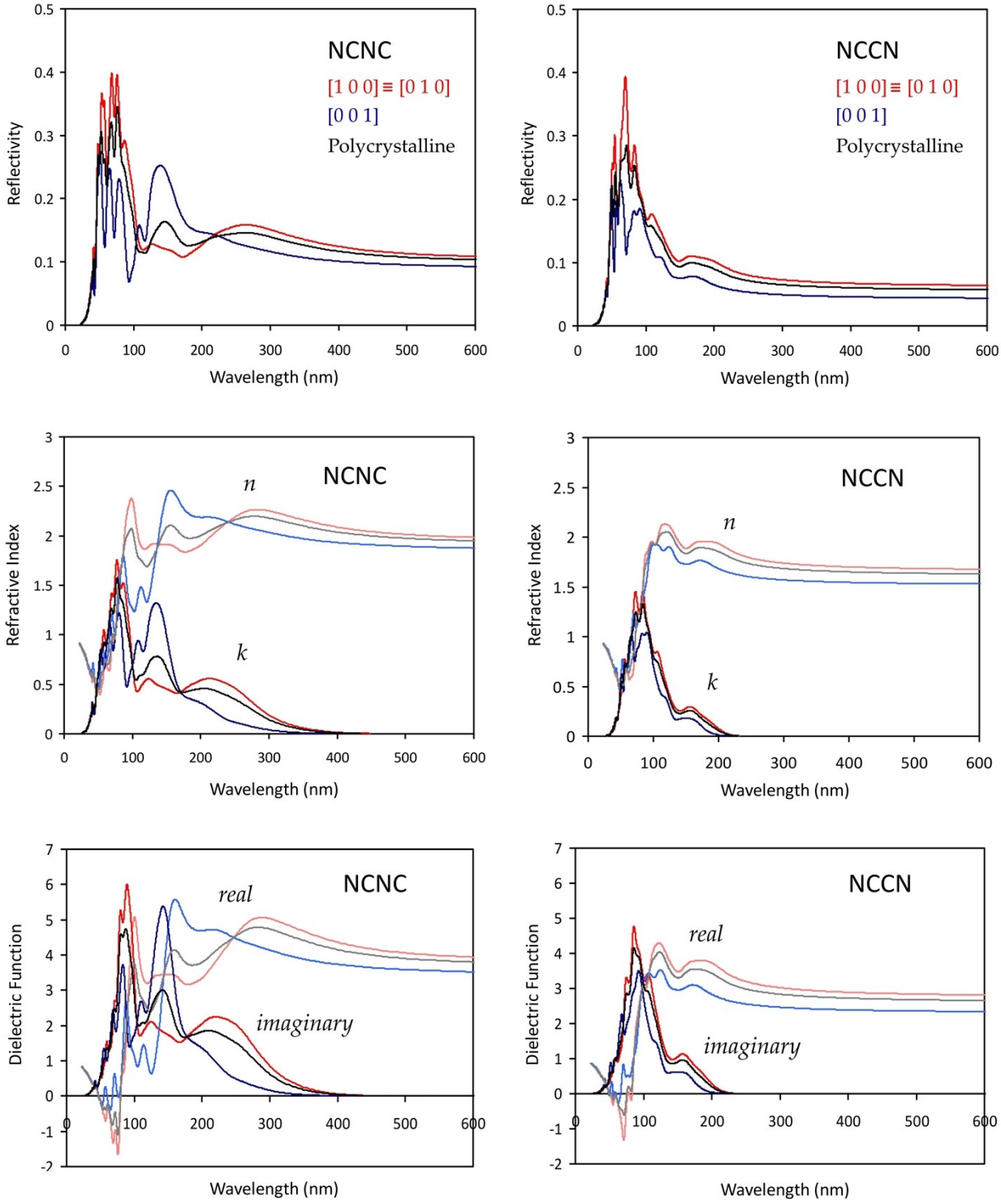

Fig. S3. The calculated optical properties: (reflectivity, refractive index and dielectric function) of the **NCNC** and **NCCN** carbon nitride phases.

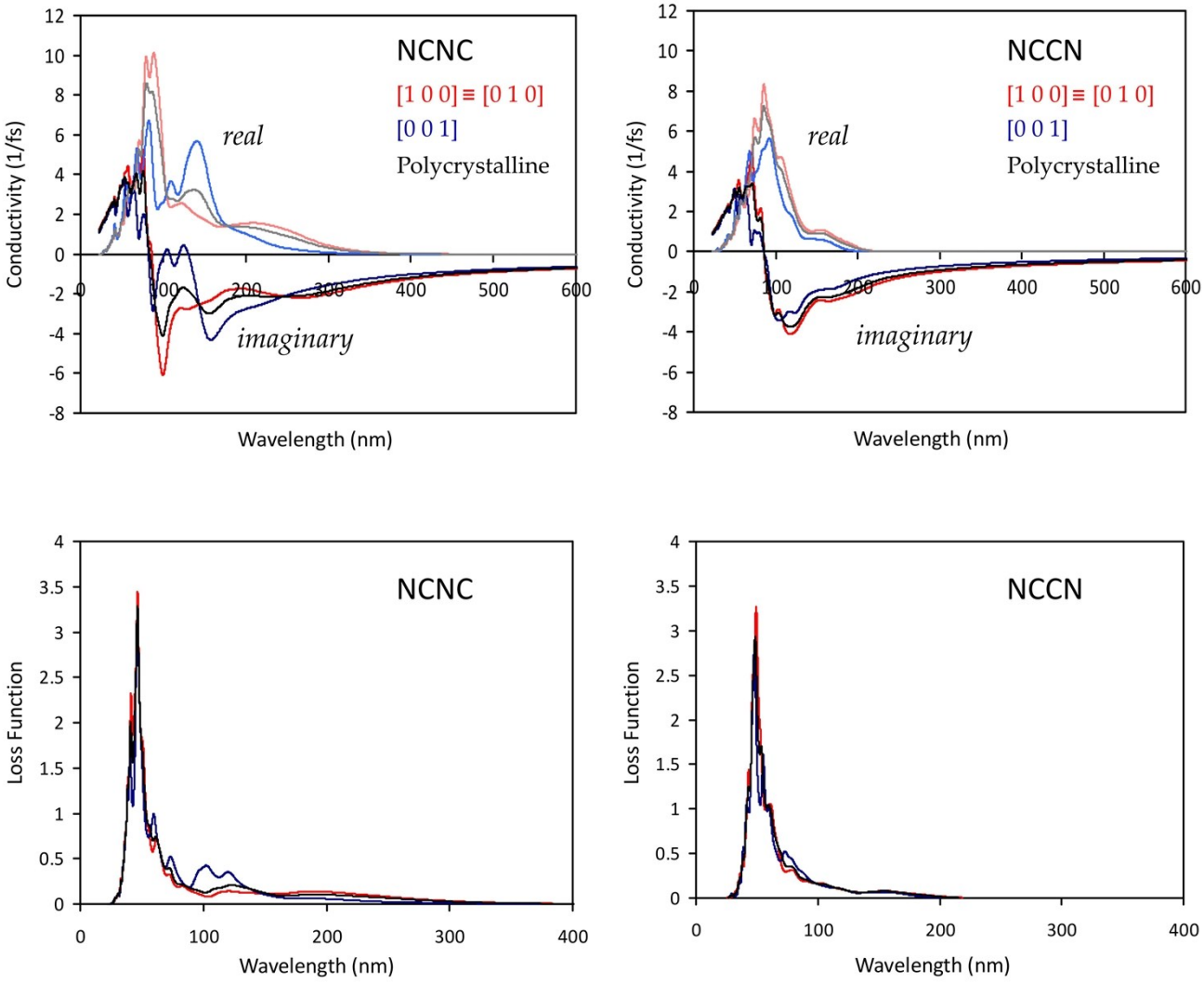

Fig. S4. The calculated optical properties: (conductivity and loss function) of the **NCNC** and **NCCN** carbon nitride phases.

Table S1. The calculated elastic stiffness constants C_{ij} (GPa). Blank corresponds to a zero value.

NCNC						
C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
1	929.20240	101.65015	2.99450	10.03120		
2	101.65015	929.20240	2.99450	-10.03120		
3	2.99450	2.99450	73.27695			
4	10.03120	-10.03120		36.98800		
5					36.98800	10.03120
6					10.03120	413.77612
NCCN						
C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
1	965.75005	106.66320	-10.11080	26.35170		
2	106.66320	965.75005	-10.11080	-26.35170		
3	-10.11080	-10.11080	58.58310			
4	26.35170	-26.35170		10.47895		
5					10.47895	26.35170
6					26.35170	429.54343

Table S2. The calculated elastic compliance constants S_{ij} (1/GPa). Blank corresponds to a zero value.

NCNC						
S_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
1	0.0010933	-0.0001230	-0.0000397	-0.0003299		
2	-0.0001230	0.0010933	-0.0000397	0.0003299		
3	-0.0000397	-0.0000397	0.0136501			
4	-0.0003299	0.0003299		0.0272147		
5					0.0272147	-0.0006598
6					-0.0006598	0.0024328
NCCN						
S_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
1	0.0011559	-0.0002204	0.0001615	-0.0034612		
2	-0.0002204	0.0011559	0.0001615	0.0034612		
3	0.0001615	0.0001615	0.0171255			
4	-0.0034612	0.0034612		0.1128373		
5					0.1128373	-0.0069224
6					-0.0069224	0.0027527

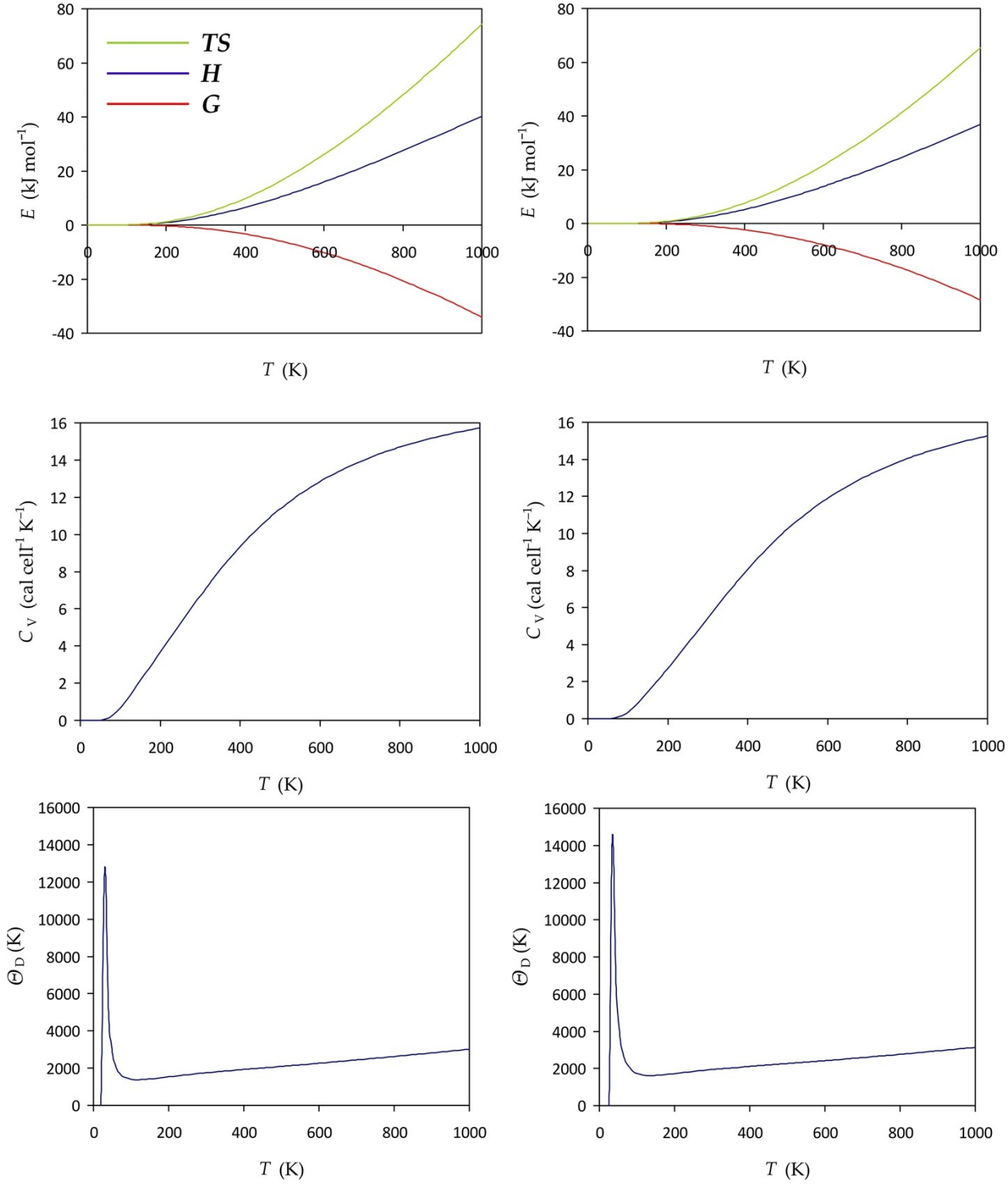

Fig. S5. Temperature dependence of thermodynamic properties of the **NCNC** and **NCCN** polymorphs.

Table S3. The QTAIM parameters (a.u.) of the symmetry-unique CPs in the NCNC polymorph

Symmetry	Multiplicity	Type	*x*	*y*	*z*	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
C_S	3	(3,-1)	0.835	0.165	0.015	0.0082984000	0.0243978000
C_{3v}	1	(3,-1)	0.333	0.667	0.483	0.2974520000	-0.1344660000
C_S	3	(3,-1)	0.527	0.473	0.693	0.3536340000	-0.5310920000
C_S	3	(3,-1)	0.189	0.378	0.321	0.4070500000	-0.7818210000
C_S	3	(3,1)	0.665	0.335	0.061	0.0068674100	0.0164989000
C_S	3	(3,1)	0.590	0.410	0.052	0.0070375200	0.0257547000
C_{3v}	1	(3,1)	1.000	0.000	0.977	0.0072020600	0.0193737000
C_S	3	(3,1)	0.058	0.114	0.980	0.0072684800	0.0235467000
C_S	3	(3,1)	0.836	0.672	0.501	0.0370790000	0.1671270000
C_{3v}	1	(3,1)	0.667	0.333	0.322	0.0414810000	0.1974350000
C_1	6	(3,3)	0.336	0.670	0.012	0.0043434100	0.0165498000
C_1	6	(3,3)	0.657	0.323	0.061	0.0068660000	0.0225821000
C_S	3	(3,3)	0.669	0.331	0.061	0.0068673300	0.0189736000
C_1	6	(3,3)	0.991	0.992	0.977	0.0072015900	0.0220290000

Table S4. The QTAIM parameters (a.u.) of the symmetry-unique CPs in the NCCN polymorph

Symmetry	Multiplicity	Type	*x*	*y*	*z*	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
C_{2h}	(3,-1)	3	0.833	0.167	0.000	0.0067983700	0.0173813000
D_{3d}	(3,-1)	1	0.333	0.667	0.500	0.3323440000	-0.4376030000
C_S	(3,-1)	6	0.042	0.521	0.676	0.3910620000	-0.6635830000
C_S	(3,1)	6	0.848	0.924	0.965	0.0057826900	0.0221696000
C_{2h}	(3,1)	3	0.833	0.667	0.500	0.0408625000	0.1914740000
C_{3v}	(3,1)	2	0.000	0.000	0.675	0.0412021000	0.1985720000
D_{3d}	(3,3)	1	0.333	0.667	0.000	0.0035309300	0.0101618000

Table S5. The QTAIM parameters of the symmetry-unique CPs in graphite

Symmetry	Type	Multiplicity	*x*	*y*	*z*	ρ (a.u.)	$\nabla^2\rho$ (a.u.)
D_{3d}	(3,-1)	2	0.000	0.000	0.000	0.0053593000	0.0157050000
C_{2v}	(3,-1)	6	0.833	0.167	0.250	0.3012690000	-0.9313060000
C_{2h}	(3,1)	6	0.500	0.500	1.000	0.0037584000	0.0124810000
D_{3h}	(3,1)	2	0.333	0.667	0.250	0.0225415000	0.1330970000
C_{3v}	(3,3)	4	0.333	0.667	0.028	0.0031275200	0.0123639000

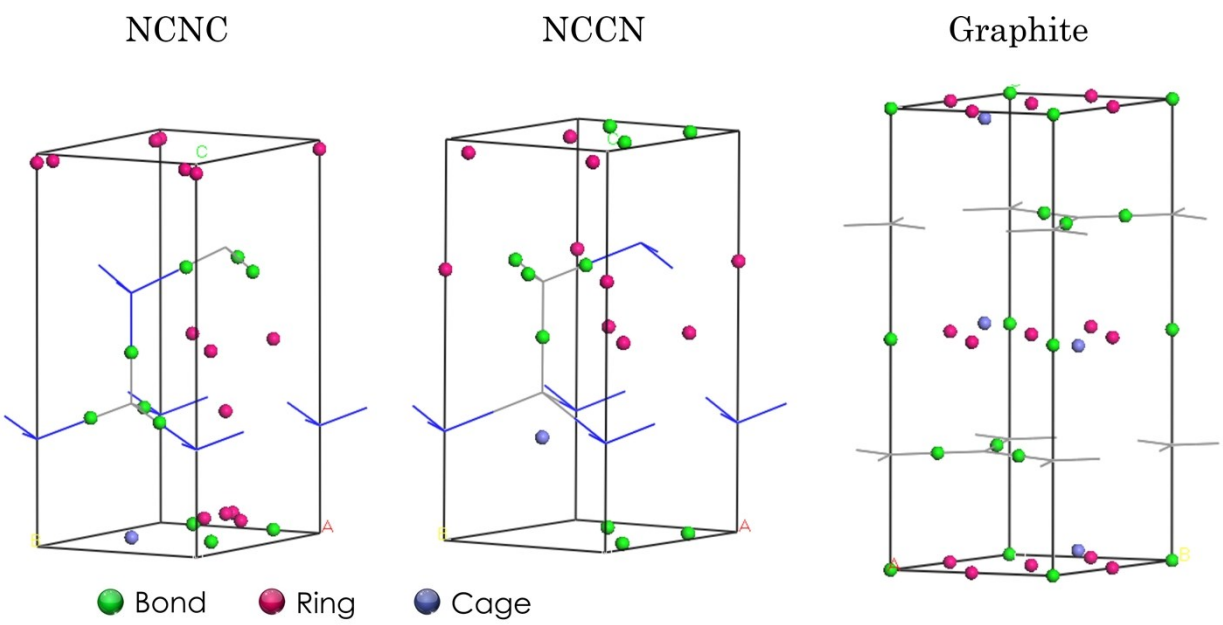

Fig. S6. Positions of the critical points in asymmetric cells of **NCNC**, **NCCN** and graphite.