Super High-Energy Density Single-Bonded Trigonal Nitrogen Allotrope—A Chemical Twin of Cubic Gauche Form of Nitrogen

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SUPPORTING INFORMATION

Physical Chemistry Chemical Physics

LIST OF SUPPLEMENTARY FIGURES AND TABLES:

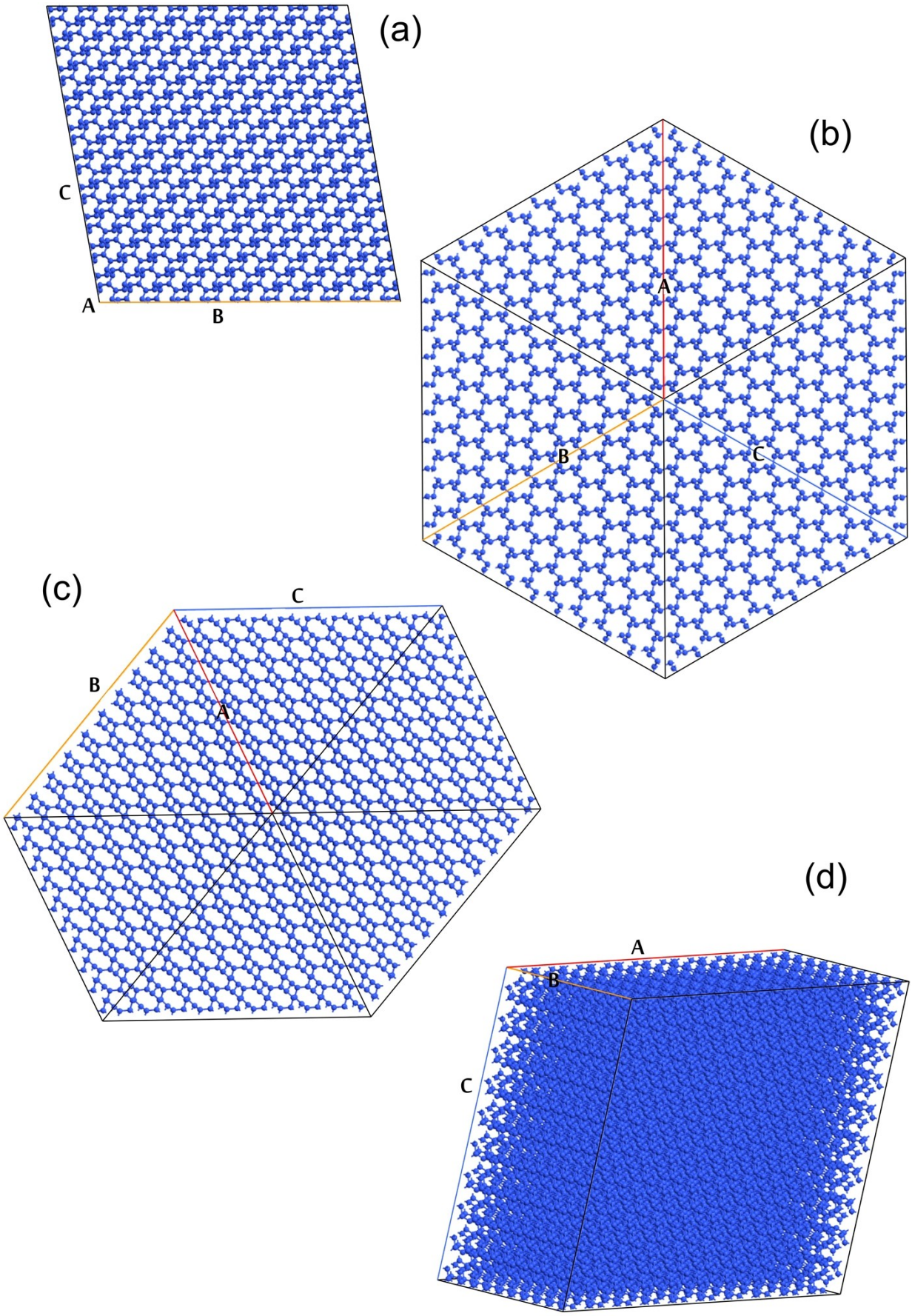


Figure S1. Different projections of a 10 × 10 × 10 unit cells slab of the **TrigN** allotrope.

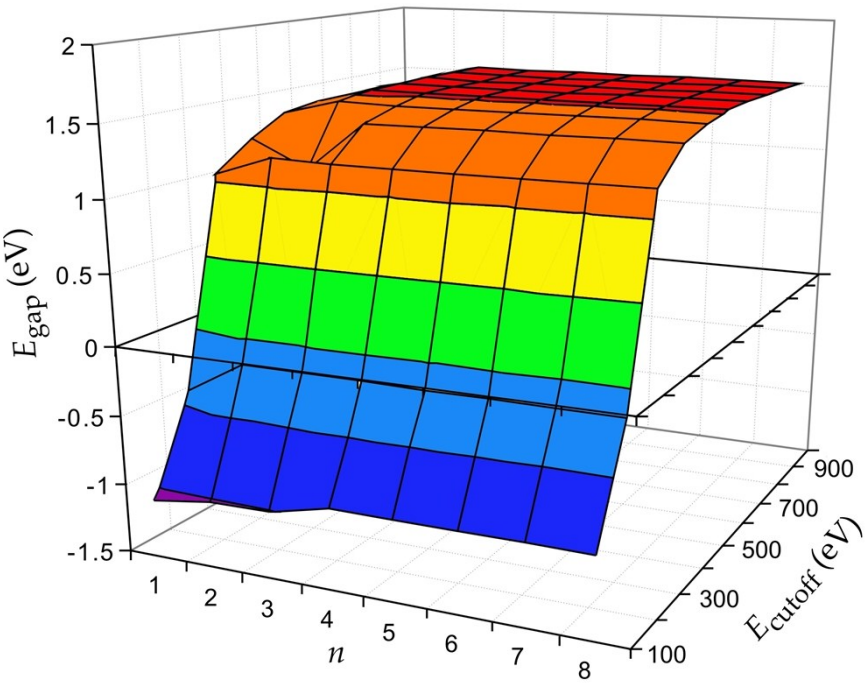


Figure S2. Dependence of the band gap obtained using NCP/PBE-TS approach on the cutoff energy and *k*-point sampling.

Table S1. The effect of cutoff energy and *k*-point sampling on the calculated band gap values

***E* (eV)**	***n* = 1**	***n* = 2**	***n* = 3**	***n* = 4**	***n* = 5**	***n* = 6**	***n* = 7**	***n* = 8**
100	-1.084	-1.021	-1.008	-0.913	-0.912	-0.912	-0.912	-0.912
200	-0.411	-0.168	-0.170	-0.170	-0.170	-0.171	-0.172	-0.172
300	1.051	1.188	1.177	1.178	1.177	1.177	1.178	1.178
400	1.239	1.046	1.398	1.399	1.399	1.399	1.399	1.399
500	1.371	1.479	1.471	1.472	1.472	1.472	1.472	1.472
600	1.413	1.518	1.51	1.511	1.511	1.511	1.511	1.511
700	1.417	1.522	1.514	1.515	1.515	1.515	1.515	1.515
800	1.417	1.522	1.514	1.515	1.515	1.515	1.515	1.515
900	1.418	1.524	1.516	1.517	1.517	1.517	1.517	1.517
1000	1.419	1.524	1.517	1.517	1.517	1.517	1.517	1.517

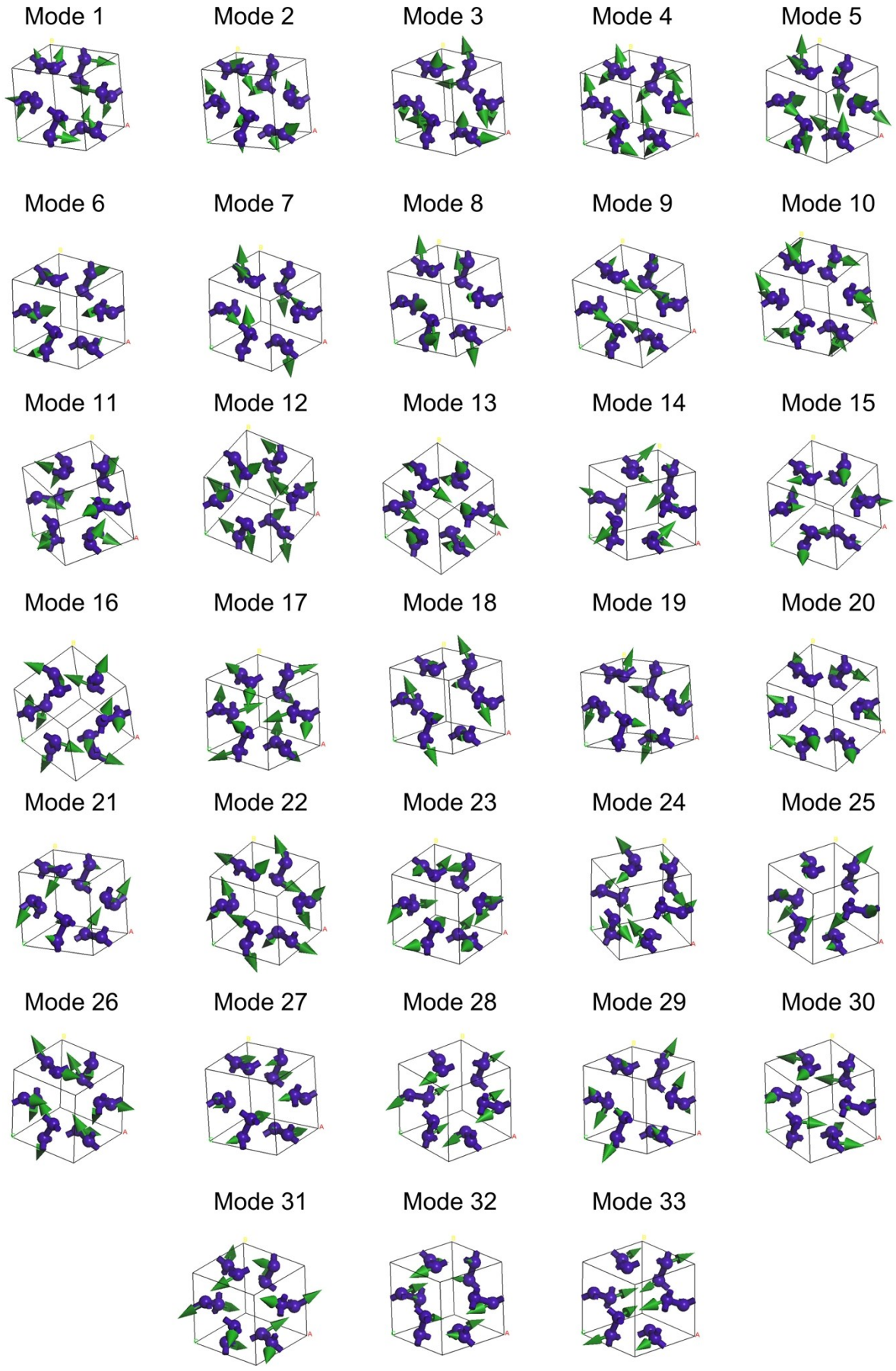
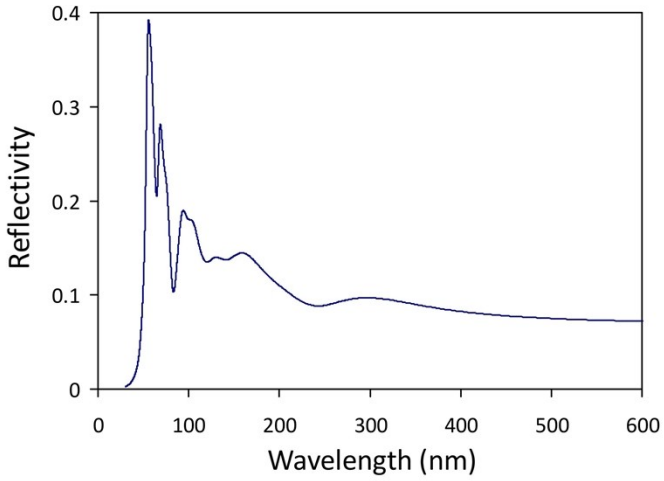
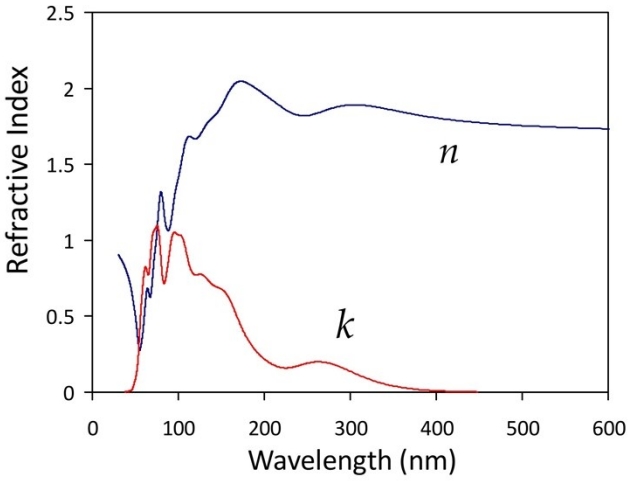
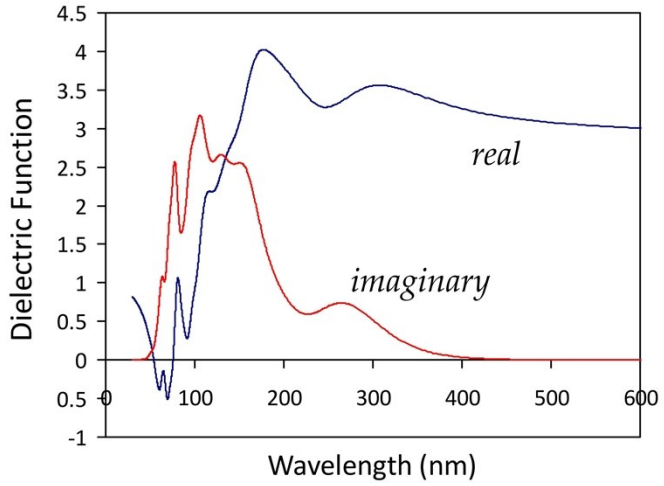
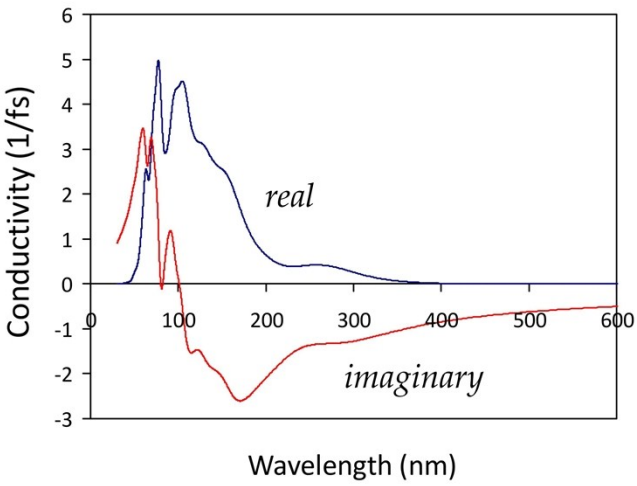


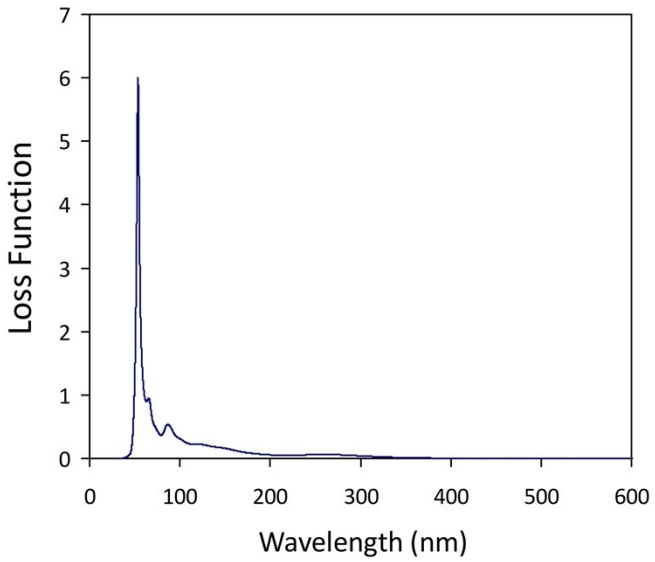
Figure S3. Graphical description of the vibrational modes in the calculated spectrum of the **TrigN** allotrope.











Reflectivity

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

Refractive Index

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

Conductivity

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

Loss Function

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

Figure S4. The calculated optical properties of the **TrigN** nitrogen allotrope.

Table S2. The calculated elastic stiffness constants C_{ij} (GPa) of the TrigN allotrope

C_{ij}	1	2	3	4	5	6
1	324.30270	88.19555	98.55745	44.18150	-18.28535	0.00000
2	88.19555	324.30270	98.55745	-44.18150	18.28535	0.00000
3	98.55745	98.55745	832.84335	0.00000	0.00000	0.00000
4	44.18150	-44.18150	0.00000	273.98975	0.00000	18.28535
5	-18.28535	18.28535	0.00000	0.00000	273.98975	44.18150
6	0.00000	0.00000	0.00000	18.28535	44.18150	118.05358

Table S3. The calculated elastic compliance constants S_{ij} (1/GPa) of the TrigN allotrope

S_{ij}	1	2	3	4	5	6
1	0.0035635	-0.0009940	-0.0003041	-0.0007349	0.0003042	0.0000000
2	-0.0009940	0.0035635	-0.0003041	0.0007349	-0.0003042	0.0000000
3	-0.0003041	-0.0003041	0.0012727	-0.0000000	0.0000000	-0.0000000
4	-0.0007349	0.0007349	0.0000000	0.0039274	-0.0000000	-0.0006083
5	0.0003042	-0.0003042	-0.0000000	-0.0000000	0.0039274	-0.0014698
6	0.0000000	0.0000000	-0.0000000	-0.0006083	-0.0014698	0.0091150

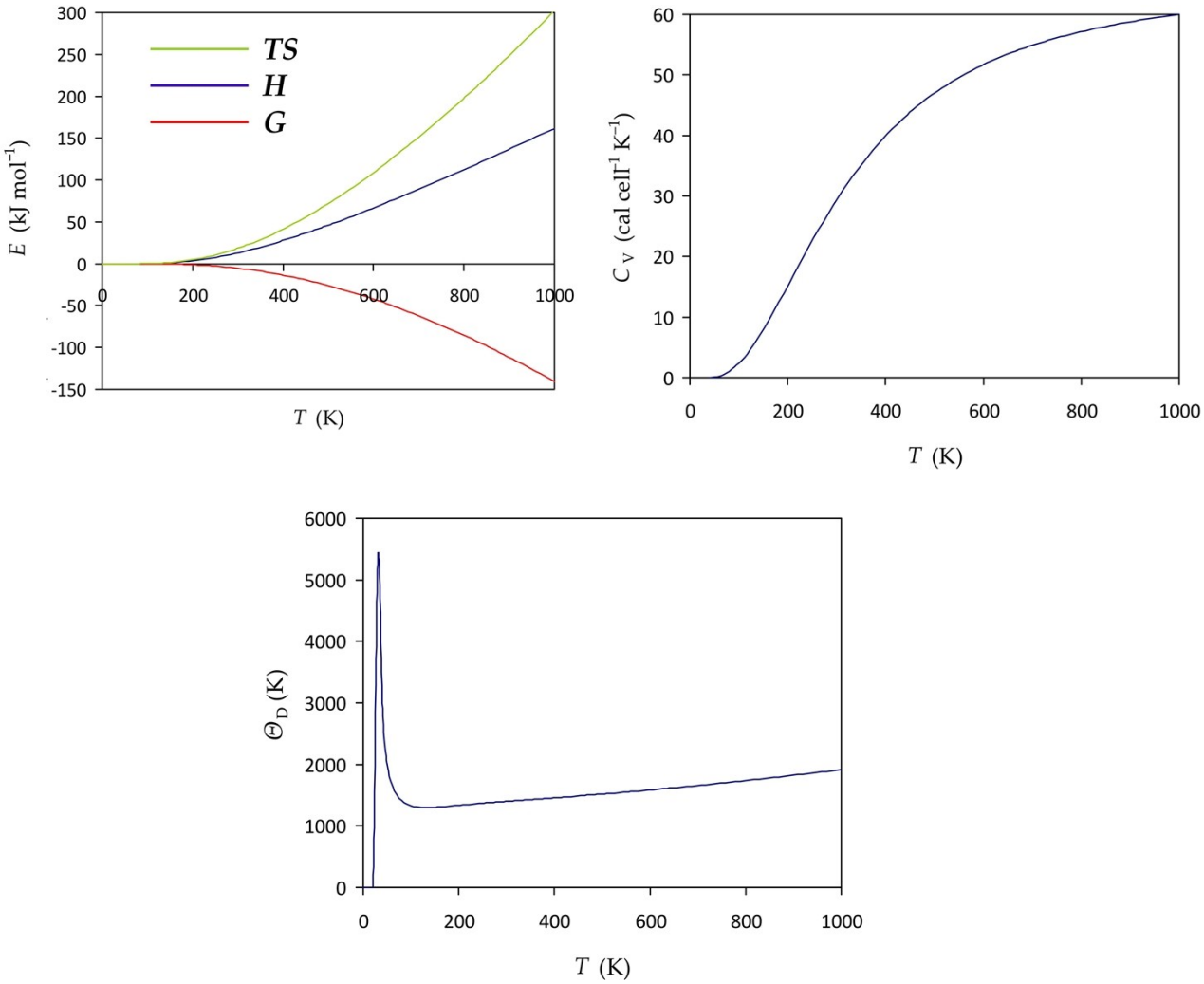


Figure S5. Temperature dependence of thermodynamic properties of the **TrigN** allotrope.