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Article

High-Throughput Screening of Dense Boron Nitride Structures from Structural Templates

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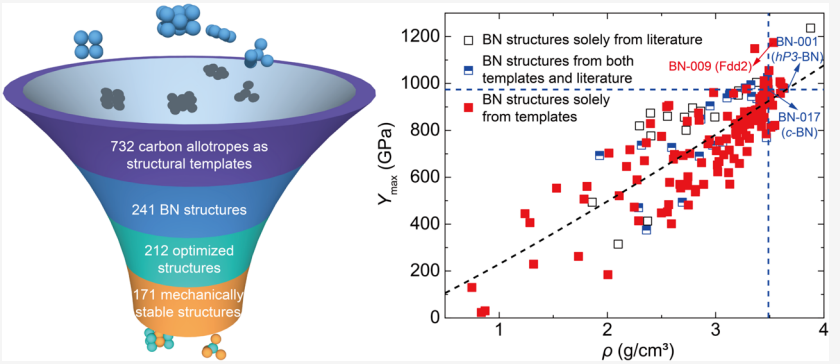

ABSTRACT: Considerable effort has been devoted to searching for high-performance boron nitride (BN) structures due to their promising applications competing with diamond. However, this search remains a significant challenge due to the exceedingly complex energy landscape of BN. Considering that most BN structures have a structure analogous to that of carbon, such as cubic BN to diamond, hexagonal BN to graphite, and that far more carbon allotropes than BN structures have been reported, we here collected 732 literature-reported carbon allotropes as structural templates to direct the discovery of BN structures. First-principles calculations indicate that 171 BN structures constructed from the carbon templates are mechanically stable, among which 139 are newly found and 32 have been reported. A literature survey shows that the number of known mechanically stable BN structures has more than tripled, indicating that our template-directed search dramatically extends the family of BN structures. Most interestingly, 15 mechanically and thermodynamically stable BN structures have a density higher than *c*-BN, and 13 of them are newly found, including the stiffest and strongest BN structures. Finally, the mechanisms and possible synthesis of high-performance BN structures are discussed.

INTRODUCTION

Light main group elements (B, C, N, *etc.*) that can form strong covalent bonds and possess high valence electron density are considered the most promising candidates for high-performance solids.[1−5] Among these elements, carbon allotropes, including carbon nanotubes, graphene, and diamond, have been extensively studied because of their impressive mechanical properties.[1−3] For instance, diamond has been long known as the hardest material and is widely used for cutting tools.[6] However, the easy reaction of diamond with ferrous metals limits the application. As a structure analogous to diamond and the second hardest material, cubic boron nitride (*c*-BN) has excellent chemical resistance to Fe-, Co-, and Ni-containing materials.[7,8] Compared to diamond, BN's chemical resistance makes it an ideal choice for cutting and drilling tools, as *c*-BN can cut all ferrous metals, including superalloys.[9,10] Additionally, BN outperforms diamond in thermal stability and oxidation temperatures, making it a promising material for a wide range of applications.[11] BN is increasingly being used in advanced electronic and optoelectronic devices. Its potential as an environmentally friendly and cost-effective material for next-generation thermoelectric devices further highlights BN's growing importance in sustainable technologies.[12,13] Hence, ultrahigh-performance BN structures are promising to compete with diamond in industrial applications.

Driven by such promising uses competing with diamond, significant efforts have been devoted to the discovery of high-performance BN structures over the past decades. Since Wentorf and Bundy first reported the transformation of hexagonal BN (*h*-BN) to *c*-BN and wurtzite BN (*w*-BN) at high pressures in the 1950s and 1960s,[14−16] the prediction, synthesis, and characterization of BN structures have been

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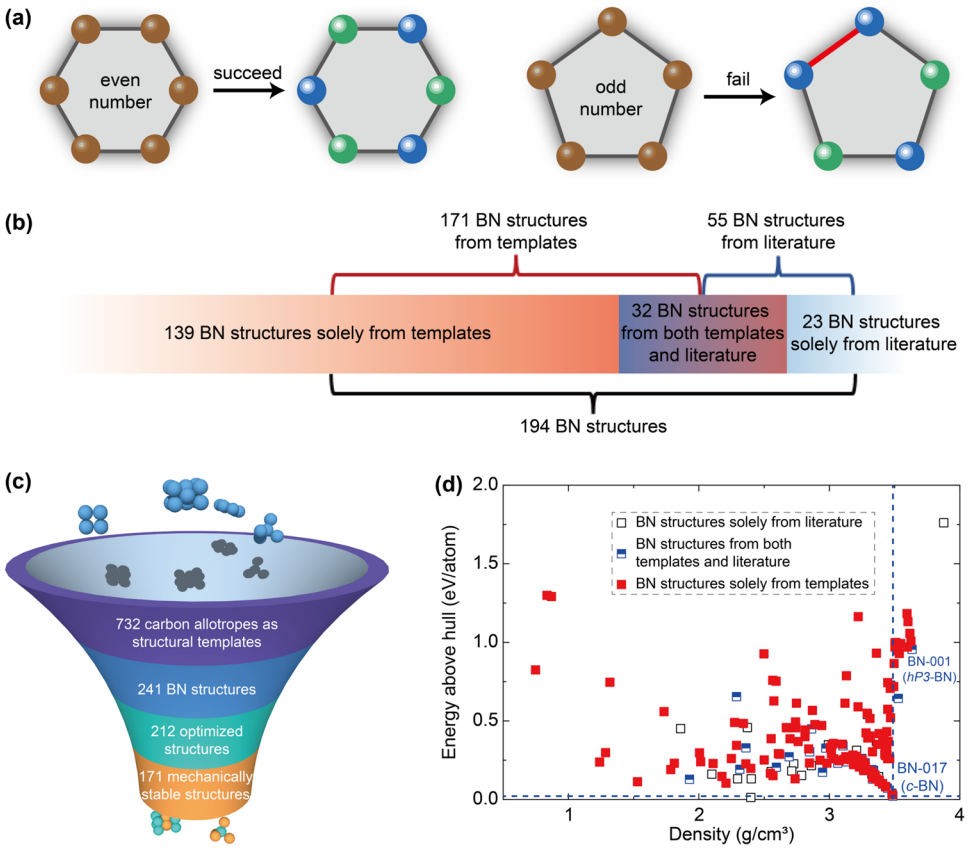

Figure 1. Screening of BN structures. (a) Illustration of atomic replacement from carbon templates, (b) mechanically stable BN structures obtained from our screening and literature, and (c) screening of mechanically stable BN structures. (d) Energies above hull for 194 mechanically stable BN structures from templates and literature.

stimulated.[17−21] First-principles calculations provide a powerful tool for materials discovery. For instance, Kuzubov et al.[22] predicted that *hP3*-BN has the highest density up to 3.66 g/cm^3, and Xiong et al.[23] predicted that *Pm3n*-BN has the highest tensile strength up to 121 GPa. Furthermore, the development of structure prediction techniques, e.g., Crystal structure AnaLYsis by Particle Swarm Optimization (CALYPSO) code,[24] has accelerated the discovery of BN structures. By employing a microhardness model,[25,26] Li et al.[27] predicted that *Pbca* (60 GPa), *Z*′-BN (60 GPa), *M*-BN (59 GPa), and BC_8-BN (57 GPa) exhibit hardness comparable to *c*-BN (63 GPa) and *w*-BN (63 GPa). Meanwhile, Zhou et al.[28] predicted that the bulk moduli of *bct*-BN (379 GPa), bct_2W_1 (383 GPa), bct_1W_1 (388 GPa), and bct_2W_2 (388 GPa) are comparable to *c*-BN (404 GPa) and *w*-BN (403 GPa). These predictions provide guidelines for the experimental syntheses of BN structures.

Most BN structures have a structure analogous to that of carbon, such as *c*-BN to diamond, and *h*-BN to graphite. Despite the progress made in the discovery of BN structures, the number of known BN structures remains significantly smaller than carbon allotropes. Our literature survey shows that only 55 unique mechanically stable BN structures have been reported, whereas the Samara Carbon Allotrope Database (SACADA) has collected 703 known carbon allotropes[29] by April 2023. The most stable stoichiometric ratio of BN structures is B:N = 1:1,[30] and the B−N bonds in BN structures exhibit bonding characteristics similar to those of C−C bonds in carbon. Considering this fact, utilizing existing carbon allotropes as structural templates holds significant potential to accelerate the discovery of BN structures.[31]

In this work, 732 carbon allotropes reported in the literature are used as templates for constructing BN structures. Screening based on first-principles calculations yields 171 mechanically stable BN structures, including 139 new and 32 known BN structures. To the best of our knowledge, the number of known stable BN structures has more than tripled, increasing from 55 to 194. Most interestingly, 15 mechanically and thermodynamically stable BN structures from templates have a density higher than *c*-BN, and 13 of them are newly found, including the stiffest BN-009 (*Fdd*2). Tensile tests show that the densest BN-001 (*hP3*-BN) has the highest recorded tensile strength. The mechanisms and possible synthesis of high-performance BN structures are discussed.

METHODS

To investigate the stabilities and mechanical properties of BN structures, first-principles calculations based on the density functional theory (DFT) were performed by using the Vienna *Ab-Initio* Simulation Package (VASP).[32] The Perdew−Burke−Ernzerhof parametrization of the generalized gradient approximation was used for the exchange-correlation functional.[33] An energy cutoff of 520 eV was used, and a *k*-point mesh with a density of about 50 Å (the product of each lattice constant and the corresponding number of *k*-points) for structural optimization and about 33 Å for elasticity tensors calculation was used for Brillouin zone sampling.[34] All structures were fully relaxed using a conjugate gradient algorithm with a

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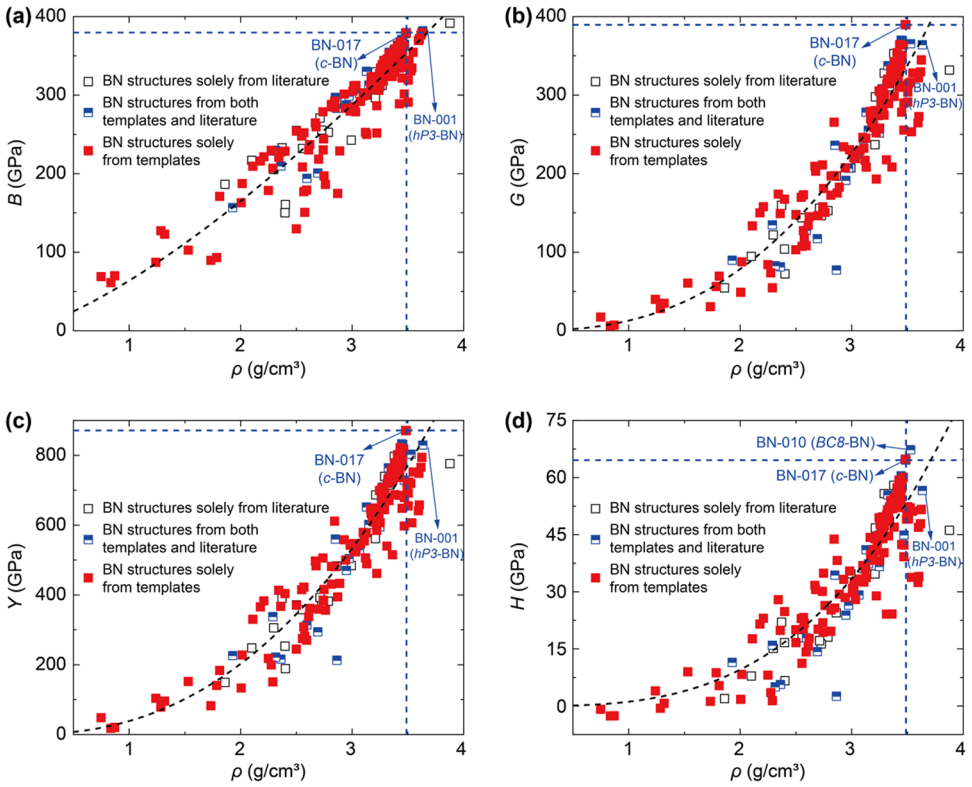

Figure 2. Performance of BN structures. (a) Bulk moduli, (b) shear moduli, (c) Young's moduli, and (d) Vickers hardness vs densities for 194 BN structures.

stringent convergence criterion of the force on each atom (10^{-3} eV/Å). In *ab initio* molecular dynamics (AIMD) simulations, an energy cutoff of 400 eV was used for a balance between computational accuracy and cost. The AIMD simulations were performed in a supercell (no less than 48 atoms) in the canonical ensemble using the Andersen thermostat.[35]

RESULTS AND DISCUSSION

Screening of Stable BN Structures. Numerous carbon allotropes have been reported in the past decades. Hoffmann et al.[29] gathered together the known carbon allotropes and indexed them in the SACADA. Meanwhile, Zhang et al.[36] recently discovered numerous superdense carbon allotropes. High-throughput screening methods have been widely used to explore novel materials.[37−43] These methods provide effective ways to explore mechanically and thermodynamically stable structures. Accordingly, we extracted 732 carbon structures from the SACADA[29] and Zhang's work[36] as templates for constructing BN structures. Subsequently, all the carbon atoms in these carbon templates were replaced with boron and nitride atoms, and the resultant structures without stable stoichiometric ratio of BN structures (B:N = 1:1) were filtered out (Figure 1a). Considering the computational efficiency, structures with more than 40 atoms in the primitive cell were further filtered out. As a result, 241 BN structures were retained for further structural optimization using first-principles calculations. Duplicate checking was then performed on these optimized structures using symmetry comparison, local atomic geometries, and structural mapping techniques to ensure uniqueness.[44] Additionally, BN structures with low-dimensional building blocks were removed using the topology-scaling algorithm proposed by Ashton et al.[45] Such screening yields 212 three-dimensional energy-optimized BN structures. To evaluate their mechanical stabilities, elasticity tensors were calculated for these 212 structures using the strain−stress method.[46] The elasticity tensors for 171 structures are positive-definite, indicating their mechanical stabilities. The screening processes are illustrated in Figure 1b,c.

A literature survey identified 60 unique BN structures from experiments and computations. To ensure consistency, we optimized these structures and assessed their mechanical stabilities using first-principles calculations. Our calculations show that 55 of the BN structures reported in the literature are mechanically stable. Upon structural checking,[44] we found that 32 mechanically stable BN structures obtained from templates were also reported in the literature, which were named "BN structures from both templates and literature" (Figure 1b). The remaining 23 mechanically stable BN structures were solely reported in the literature, which were named "BN structures solely from literature". This indicates that 139 BN structures obtained from templates are newly found compared to the 55 structures reported in the literature (Figure 1b). These 139 newly found BN structures were named "BN structures solely from templates". These results demonstrate that template-directed search dramatically extends the family of BN structures, since the number of known stable BN structures has more than tripled (from 55 to 194). All these 194 BN structures are provided in the Supporting Information (Table S1). Formability is important for practical applications, which can be measured by energies above hull. The energies above hull of BN structures were calculated as the energy difference between the energy for a BN structure and that of the lowest energy BN (*h*-BN). The calculated energies above hull of these

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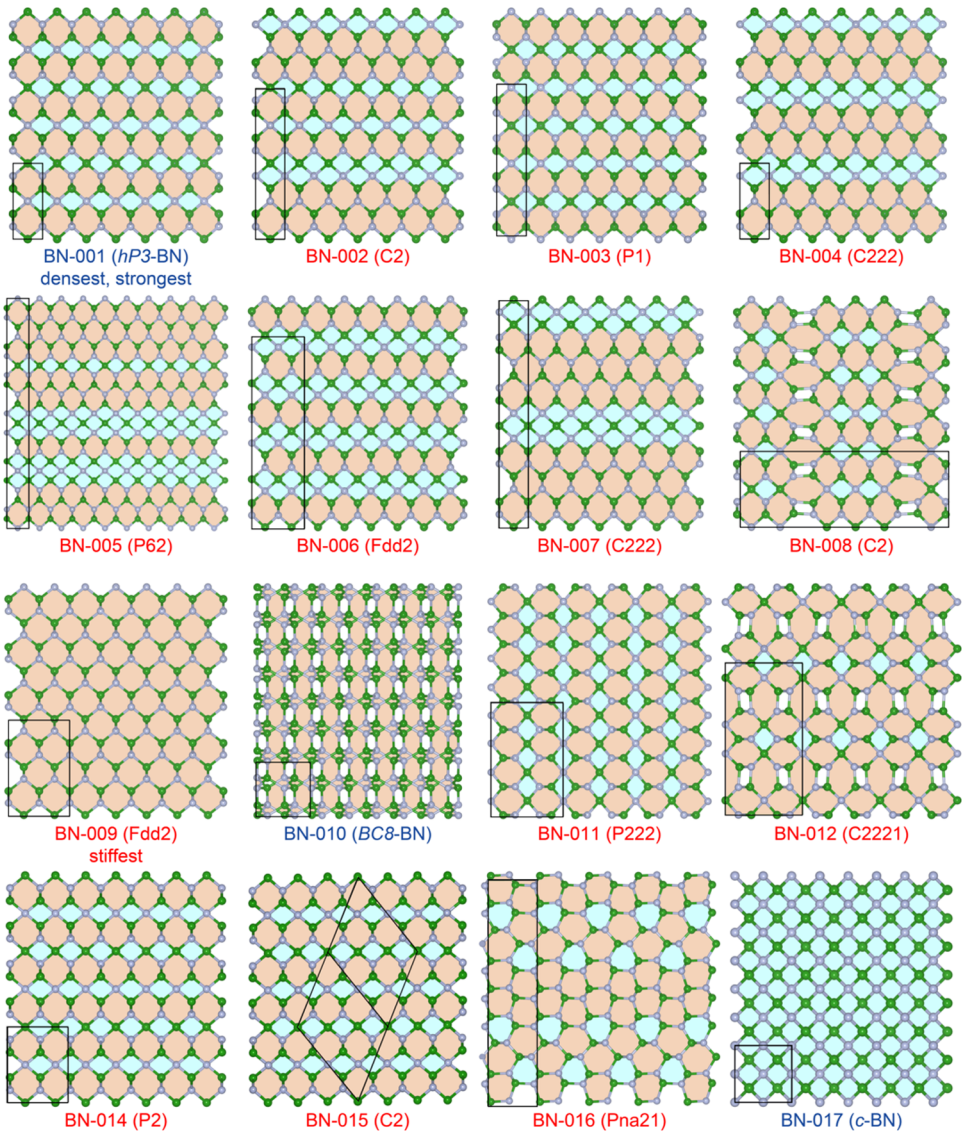

Figure 3. Stable superdense BN structures compared to *c*-BN. BN structures not reported in the literature are marked with their space groups, and the literature-reported structures are marked with their names in the literature.

194 mechanically stable BN structures are shown in Figure 1d and Table S1.

Mechanical Performance of BN Structures. We investigated the mechanical properties of these BN structures. Based on the theory of elasticity, we calculated the Voigt-Reuss-Hill average elastic moduli of BN structures.[47] Unless otherwise noted, the elastic moduli mentioned below are all based on the Voigt-Reuss-Hill averaging scheme. The bulk modulus (B), shear modulus (G), and Young's modulus (Y) can be derived from the elasticity tensor of a material (Figure 2a−c and Table S1). Elastic moduli not only characterize the resistance of a material to elastic deformation but also have a close correlation with other important properties. For example, Vickers hardness of a material can be correlated with the bulk modulus and shear modulus as $H = 2\ (G^3/B^2)^{0.585} - 3$.[48] Therefore, the hardness of these BN structures can be further estimated from their elastic moduli (Figure 2d and Table S1). As a validation, our calculated bulk modulus (380 GPa), shear modulus (390 GPa), Young's modulus (871 GPa), and Vickers hardness (65 GPa) of *c*-BN, agree well with the literature-reported corresponding values (376, 382, 856, and 65 GPa, respectively).[49,50] We identified several BN structures with novel superhard properties. These structures exhibit Vickers hardness values comparable to recently reported BN structures, such as the *Pm* BN reported by Fan et al.[51] and *O*-BN reported by Huang et al.[52] The hardness of these new BN structures could be further enhanced through nanostructuring, such as nanograined and nanotwinned microstructures, providing a general pathway for designing advanced materials with exceptional thermal stability and mechanical properties.[53,54]

We further explored the correlations between the densities and the mechanical properties. These results show that the correlation coefficients (R^2) of densities with B, G, Y, and H are as high as 0.88, 0.88, 0.89, and 0.81, respectively (Figure 2). Meanwhile, the correlation of the highest Young's modulus with the density is also strong (Figure S1). These strong correlations between the densities and the mechanical properties suggest that high density can serve as an indicator for screening high-mechanical-performance BN structures. Hence, we performed an in-depth study on BN structures with a high density in the following investigation. Unless otherwise noted, each BN structure in this work is named as

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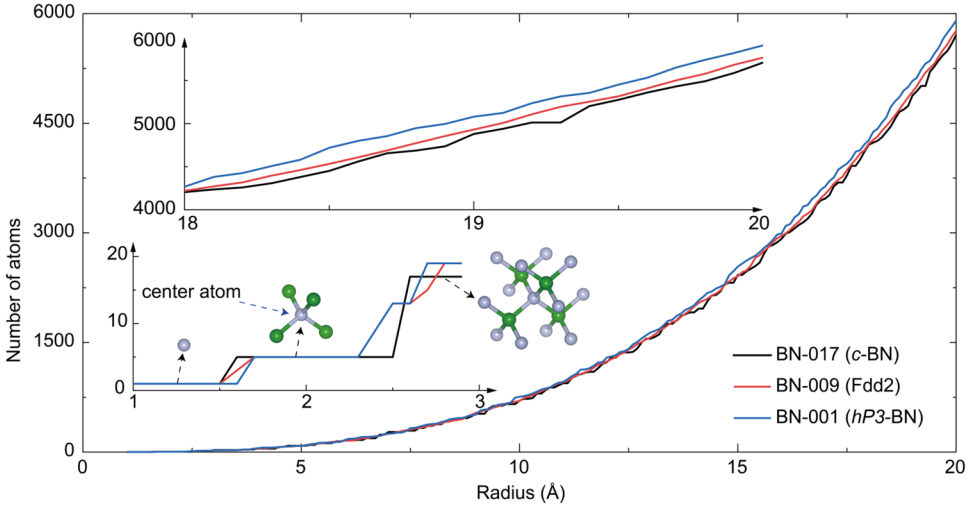

Figure 4. Superdense mechanisms of BN structures. Statistical analyses by counting the number of atoms within various spherical shells centered on each atom for BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) compared to BN-017 (*c*-BN).

"BN-number (space group)" (Table S1). Among these 194 BN structures, 17 exhibit densities exceeding that of *c*-BN and were defined as superdense BN structures. We further investigated the thermodynamic stabilities of superdense BN structures by conducting AIMD simulations for 10 ps at room temperature (300 K). The simulations show that 15 structures from templates can maintain structural integrity (Figure 3), and 13 of them are newly found in this work. In the following investigation, we refer to structures that possess both mechanical and thermodynamic stability as stable structures, and we exclusively focus on these stable superdense BN structures.

Considering the mechanical anisotropy, the direction-dependent mechanical properties are also interesting. The mechanical anisotropy of BN-009 (*Fdd*2) (the ratio of the maximum and minimum Young's modulus: Y_{max}/Y_{min} = 2.9) exceeds that of *c*-BN (Y_{max}/Y_{min} = 1.3), and BN-009 (*Fdd*2) has the highest recorded Y_{max} (1175 GPa) that is 21% larger than that of *c*-BN (974 GPa). To the best of our knowledge, no other BN structures have been identified to have a higher Y_{max} than BN-009 (*Fdd*2). Furthermore, the densest [BN-001 (*hP3*-BN)] and stiffest [BN-009 (*Fdd*2)] BN structures discovered from our template-based screening were investigated by uniaxial tensile tests along the direction of the maximum Young's modulus. Tensile tests of BN-017 (*c*-BN) and BN-122 (*Pm3n*-BN with the highest tensile strength of 121 GPa reported in literature[23]) were also performed for comparison (Figure S2). The results show that the tensile strengths for BN-017 (*c*-BN) and BN-122 (*Pm3n*-BN) in the Y_{max} direction are 59 and 117 GPa, respectively, which are generally consistent with the literature reported values (55 and 121 GPa, respectively),[20,23] while the tensile strength of BN-001 (*hP3*-BN) (172 GPa) and BN-009 (*Fdd*2) (126 GPa) significantly exceed the highest reported tensile strength of BN-122 (*Pm3n*-BN) (117 GPa). To summarize, these results demonstrate that our template-directed search has led to the discovery of the predicted stiffest BN structure [BN-009 (*Fdd*2)] and the predicted strongest BN structure [BN-001 (*hP3*-BN)].

Considering the correlations between the densities and the mechanical properties, an investigation of BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) was conducted to elucidate the mechanisms for their higher densities than BN-017 (*c*-BN). All these structures are tetrahedrally coordinated (sp^3 hybridization as shown in Figure 2). Despite their tetrahedral coordination, the tetrahedral structures of these BN variants are not identical. BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) can be regarded as distorted structures compared to BN-017 (*c*-BN). This structural distortion is reflected in the atomic distribution. To probe the atomic distribution at various neighbor levels, we performed statistical analyses by counting the number of atoms within various spherical shells centered on each atom. As shown in Figure 4, within the shell radius range of 2.8−2.9 Å, BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) accommodate 19 atoms, whereas BN-017 (*c*-BN) accommodates 17 atoms. As the shell radius increases, the difference in the number of atoms among these structures becomes more pronounced. In the range of 18−20 Å, BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) exhibit a higher number of atoms compared to BN-017 (*c*-BN). This highlights the role of structural distortions in enhancing the density of these materials. As the radius grows, the density gap continues to increase, providing a clearer distinction between these structures. This mechanism is similar to analogous carbon structures (*hP3* carbon and diamond).[55]

Additional Remarks on the Fabrication of BN Structures. The synthesis of materials is a key for applications. To synthesize BN structures, various methods can be employed, including high-temperature and high-pressure synthesis,[14,54] atmospheric pressure synthesis,[56] temperature gradient method,[57] chemical vapor deposition method,[58] and physical vapor deposition method.[59] Each method has its advantages and limitations.[12] The choice of BN precursors significantly influences the resultant BN structures. For example, onion-like BN has been used as the precursor to synthesize nanotwinned *c*-BN,[54] and *h*-BN has been used as the precursor to synthesize *c*-BN and *w*-BN.[14−16,52] *O*-BN has been predicted that it can be synthesized using BN nanotubes as the precursor.[52] These results suggest that it is possible to synthesize new BN structures through low-density, low-dimensional BN structures, such as fullerene-like BN structures,[60] and amorphous structures.[61] Our newly predicted BN structures exhibit excellent mechanical properties and hold great promise to be synthesized experimentally. These BN structures, along with their remarkable properties, show

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promising potential for various technological fields.[10,11,62−65] For example, BN-001 (*hP3*-BN) and BN-009 (*Fdd*2) exhibit fracture strains greater than 20%, making them suitable for applications in strain engineering and related fields. Moreover, the energy above hull is used to characterize the formability of a material. A low energy above hull usually indicates likely ease of synthesis for a material. Our calculated energies above hull of 194 BN structures are shown in Figure 1d and Table S1. It can be found that all the energies above hull for these BN structures from templates are below 1.4 eV/atom, and most of them are below 0.5 eV/atom, indicating their formability for applications. These results provide references for future BN syntheses.

CONCLUSIONS

In summary, we propose a template-directed searching strategy to accelerate the discovery of BN structures from complex energy landscapes. This search yields 171 unique BN structures with good mechanical stability. Among these structures, 32 BN structures have been computationally or experimentally fabricated in the literature, providing valuable support for our work. Meanwhile, the number of known mechanically stable BN structures has more than tripled, indicating that our template-directed search significantly extends the family of BN structures. Analyses of these structures show strong correlations between the densities and the mechanical properties. Most interestingly, 15 stable BN structures from templates have a density significantly higher than *c*-BN, and 13 of them are newly found, including the predicted densest and strongest BN-001 (*hP3*-BN), and the predicted stiffest BN-009 (*Fdd*2). Finally, the superdense mechanisms and possible synthesis of high-performance BN structures are discussed.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpcc.4c08627.

Highest Young's modulus (Y_{max}) vs density (ρ) for mechanically stable BN structures from the template method, tensile stress−strain curves of BN structures stretched along the direction of highest Young's modulus, and raw data of calculations and relevant literature (PDF)

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Notes

The authors declare no competing financial interest.

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Supporting Information

High-Throughput Screening of Dense Boron Nitride Structures from Structural Templates

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This supporting information contains

(1) Figures S1-S2.

(2) Table S1.

(3) Structural and mechanical information of mechanically stable BN structures.

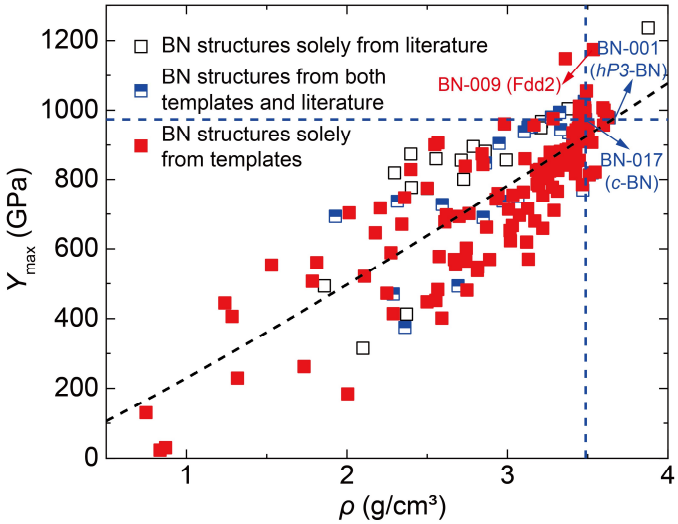

Fig. S1. Highest Young's modulus (Y_{max}) vs. density (ρ) for mechanically stable BN structures from the template method.

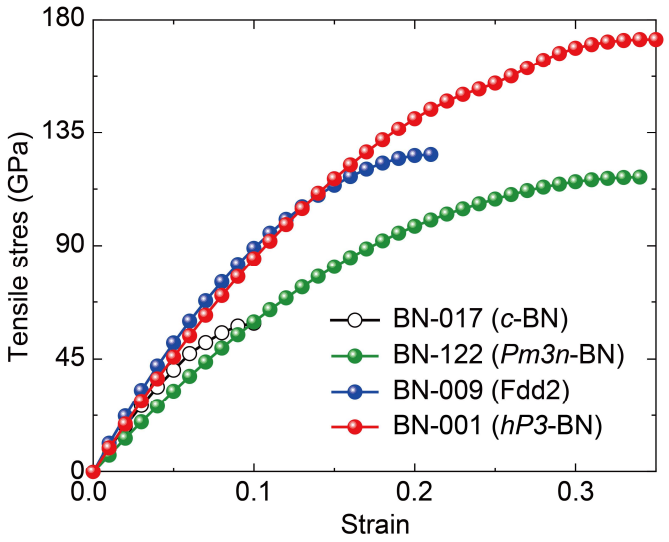

Fig. S2. Tensile stress-strain curves of BN structures stretched along the direction of highest Young's modulus.

Table. S1. Density (ρ), space group (SG), bulk modulus (B), shear modulus (G), Young's modulus (Y), highest Young's modulus (Y_{max}), Vickers hardness (H), and energy above hull of 194 mechanically stable BN structures from templates and literature. BN-001 to BN-171 are from templates, while BN-172 to BN-194 are from literature. The black represents BN structures solely from templates, the blue represents BN structures from both templates and literature, and the purple represents BN structures solely from literature.

Name	ρ (g/cm^3)	SG	B (GPa)	G (GPa)	Y (GPa)	Y_{max} (GPa)	H (GPa)	Energy above hull (eV/atom)	Notes
BN-001	3.63	181	382	364	829	979	57	0.95	*Hp*-BN; *hP3*-BN[1-2]
BN-002	3.63	5	379	345	794	981	52	1.01	
BN-003	3.63	1	379	345	794	980	52	1.01	
BN-004	3.62	21	377	330	765	982	48	1.06	
BN-005	3.60	171	372	273	658	1001	34	1.13	
BN-006	3.60	43	370	322	749	958	47	0.97	
BN-007	3.60	21	370	265	641	1007	32	1.18	
BN-008	3.55	5	354	328	752	821	51	0.99	
BN-009	3.54	43	334	253	607	1175	34	0.93	
BN-010	3.53	205	333	365	803	819	67	0.64	*BC*$_8$-BN[3]
BN-011	3.53	16	331	316	719	907	52	0.95	
BN-012	3.51	20	344	315	723	813	49	1.00	
BN-013	3.50	3	291	291	655	917	52	1.00	thermodynamically unstable
BN-014	3.50	3	319	304	692	953	51	0.97	
BN-015	3.50	5	335	313	715	913	50	0.86	
BN-016	3.49	33	336	310	711	1055	49	0.72	
BN-017	3.49	216	380	390	871	974	65	0.02	*c*-BN[3-8]
BN-018	3.48	186	379	390	871	1000	65	0.03	
BN-019	3.48	160	379	390	870	999	65	0.03	
BN-020	3.48	160	378	390	870	1007	65	0.03	
BN-021	3.48	186	379	390	871	1025	65	0.04	*w*-BN[3,5,8-10]
BN-022	3.47	220	365	312	728	769	45	0.73	*C12*-BN[11]
BN-023	3.47	29	343	290	679	938	42	0.52	
BN-024	3.47	39	301	255	597	785	39	0.71	
BN-025	3.46	33	363	364	818	924	60	0.26	
BN-026	3.45	5	354	350	790	922	58	0.37	
BN-027	3.45	7	322	278	648	855	42	0.74	
BN-028	3.45	152	351	346	782	1012	57	0.57	
BN-029	3.45	7	357	351	793	977	57	0.26	
BN-030	3.44	55	371	370	833	937	60	0.07	*O*-BN; *Pbam*-BN[12-13]
BN-031	3.44	33	354	338	768	950	54	0.28	
BN-032	3.44	4	345	342	771	929	57	0.43	
BN-033	3.44	4	350	342	774	909	56	0.31	
BN-034	3.44	33	351	342	775	909	56	0.31	
BN-035	3.44	31	348	338	767	916	55	0.33	

BN-036	3.43	58	368	364	821	928	59	0.08	3D (6,6)-III; Pnnm (58)[14]
BN-037	3.43	26	368	364	822	928	59	0.08	
BN-038	3.43	29	352	345	780	854	57	0.28	
BN-039	3.43	31	368	364	821	929	59	0.08	
BN-040	3.43	8	344	342	770	944	57	0.32	
BN-041	3.43	4	334	329	744	892	55	0.35	
BN-042	3.42	33	289	310	685	816	59	0.29	
BN-043	3.42	29	341	323	736	867	52	0.40	
BN-044	3.41	55	362	353	800	931	57	0.10	*Z*-BN; bct_1w_1; 3D (4,4)-IV; Pbam (55)[14-16]
BN-045	3.41	14	344	328	746	936	53	0.36	
BN-046	3.41	31	363	352	797	932	57	0.10	*P*-BN; bct_2w_2[15]
BN-047	3.41	61	363	354	801	896	57	0.10	
BN-048	3.38	186	358	341	777	866	54	0.12	
BN-049	3.38	62	357	342	778	887	55	0.12	
BN-050	3.38	36	358	340	776	935	54	0.11	bct_2w_1[15]
BN-051	3.38	34	329	298	687	882	47	0.42	
BN-052	3.38	29	358	342	778	888	55	0.12	
BN-053	3.37	14	338	320	729	885	52	0.35	
BN-054	3.36	36	354	334	761	880	53	0.13	
BN-055	3.36	56	324	208	515	1148	24	0.93	
BN-056	3.35	173	353	330	755	841	52	0.14	
BN-057	3.35	62	346	332	755	861	54	0.16	
BN-058	3.34	62	335	319	727	877	52	0.19	*Z*'-BN[3]
BN-059	3.33	136	354	315	729	945	47	0.13	*bct*-BN;3D (4,4)-III; P42mnm (136); *pct*-BN; *β*-BeO[3,14,17-18]
BN-060	3.33	62	341	315	723	864	50	0.17	
BN-061	3.33	14	327	289	670	880	45	0.30	
BN-062	3.33	61	352	320	736	870	49	0.14	*AW*-BN; Pbca[15]
BN-063	3.33	14	352	318	733	881	49	0.14	
BN-064	3.33	62	341	316	725	859	50	0.17	
BN-065	3.33	45	346	337	764	994	55	0.19	3D (8,0)-II; Iba2 (45)[14]
BN-066	3.32	36	337	314	719	841	50	0.16	AW_1W_1[15]
BN-067	3.32	59	340	320	731	846	52	0.18	
BN-068	3.32	2	337	315	720	826	50	0.40	
BN-069	3.31	2	346	218	540	766	24	0.52	
BN-070	3.30	14	328	299	688	876	47	0.39	
BN-071	3.29	19	329	275	644	710	40	0.55	
BN-072	3.29	38	344	305	707	976	46	0.19	
BN-073	3.28	14	318	281	651	778	44	0.42	
BN-074	3.28	62	329	307	703	829	50	0.21	
BN-075	3.27	39	338	308	709	981	48	0.23	3D (6,0)-II; Aem2 (39)[14]
BN-076	3.27	14	331	293	679	835	45	0.19	
BN-077	3.27	63	339	307	707	845	48	0.23	
BN-078	3.27	19	330	295	682	828	46	0.19	
BN-079	3.27	14	332	291	675	879	44	0.18	

BN-080	3.26	14	330	292	676	824	45	0.19	
BN-081	3.26	36	329	293	677	825	45	0.19	AW_1M_2[15]
BN-082	3.26	56	335	304	700	835	48	0.24	
BN-083	3.25	11	313	258	607	811	38	0.25	
BN-084	3.25	164	311	252	595	805	37	0.26	AW_1bct_1[15]
BN-085	3.25	60	327	305	699	813	49	0.25	
BN-086	3.24	62	307	278	641	810	45	0.25	
BN-087	3.24	55	306	274	633	804	44	0.25	
BN-088	3.23	14	320	278	647	845	43	0.21	
BN-089	3.22	17	252	193	461	752	29	1.16	
BN-090	3.22	88	286	252	585	659	41	0.59	
BN-091	3.21	59	316	280	649	803	44	0.27	
BN-092	3.20	12	313	259	608	829	38	0.23	
BN-093	3.20	14	310	267	622	782	41	0.24	
BN-094	3.19	18	310	266	620	804	41	0.23	
BN-095	3.19	14	308	261	611	787	40	0.22	
BN-096	3.18	121	318	266	623	826	39	0.28	
BN-097	3.17	15	323	270	633	679	40	0.27	
BN-098	3.17	41	313	279	646	958	44	0.25	
BN-099	3.15	44	313	255	602	954	37	0.26	*I*-BN[19]
BN-100	3.13	88	250	208	489	570	34	0.79	
BN-101	3.13	108	330	278	652	952	41	0.24	3D (8,0)-I; I4cm (108)[14]
BN-102	3.13	114	300	245	578	716	36	0.27	
BN-103	3.12	88	253	217	506	619	36	0.61	
BN-104	3.11	62	303	232	555	860	33	0.25	
BN-105	3.11	187	301	244	577	939	36	0.34	*H18*-BN[13]
BN-106	3.10	121	299	246	579	763	37	0.35	
BN-107	3.08	60	292	230	546	696	33	0.25	
BN-108	3.07	62	302	219	530	750	29	0.23	*M2*-BN; *Pnma*-BN; *III*-BN[14-15]
BN-109	3.03	62	312	219	533	755	28	0.26	
BN-110	3.03	94	279	220	523	667	33	0.36	
BN-111	3.02	81	286	220	525	623	32	0.34	
BN-112	3.02	130	312	226	547	652	30	0.29	
BN-113	3.01	36	305	227	546	713	31	0.33	
BN-114	2.98	87	280	230	542	961	35	0.23	
BN-115	2.97	87	299	207	504	737	26	0.33	3D (4,4)-II; I4m (87)[14]
BN-116	2.95	71	287	191	470	904	24	0.17	3D(6,6)-IV; Immm[14]
BN-117	2.94	138	283	207	500	760	28	0.47	
BN-118	2.93	176	301	234	558	743	33	0.25	
BN-119	2.89	57	229	183	433	570	29	0.48	
BN-120	2.87	36	175	175	394	662	38	0.57	
BN-121	2.86	21	283	77	213	848	3	0.45	*T*-B_7N_7[8]
BN-122	2.85	223	297	236	560	690	34	0.30	*Pm3n*-BN[20]
BN-123	2.85	189	284	197	481	843	26	0.23	
BN-124	2.84	184	292	265	611	874	44	0.32	
BN-125	2.82	8	288	197	482	548	25	0.44	

BN-126	2.81	217	285	173	431	537	20	0.40	
BN-127	2.76	18	186	151	356	701	26	0.37	
BN-128	2.75	36	197	181	416	481	35	0.61	
BN-129	2.74	70	244	155	383	602	19	0.46	
BN-130	2.74	126	230	158	385	565	22	0.49	
BN-131	2.74	185	279	211	506	839	30	0.13	
BN-132	2.70	129	218	146	359	692	20	0.39	
BN-133	2.69	156	201	117	294	493	14	0.27	*Rh6*-BN[21]
BN-134	2.68	165	260	203	483	554	31	0.46	
BN-135	2.67	216	265	209	497	570	32	0.46	
BN-136	2.62	57	237	145	362	697	18	0.29	
BN-137	2.61	72	230	134	337	677	16	0.29	
BN-138	2.59	46	194	128	314	727	18	0.21	*dz2*-BN; *O16*-BN[11,22]
BN-139	2.59	111	179	108	270	401	14	0.75	
BN-140	2.58	136	151	119	282	578	22	0.63	
BN-141	2.57	38	252	173	422	906	23	0.15	
BN-142	2.57	136	177	128	309	483	20	0.76	
BN-143	2.55	5	209	107	275	452	11	0.39	
BN-144	2.55	127	248	170	415	900	23	0.17	
BN-145	2.50	105	254	147	371	775	17	0.25	
BN-146	2.50	121	130	103	245	448	20	0.93	
BN-147	2.40	145	229	167	404	829	25	0.20	
BN-148	2.36	122	210	81	216	375	6	0.33	*cT8*-BN[23]
BN-149	2.36	160	227	149	367	747	20	0.23	
BN-150	2.34	35	221	174	413	670	28	0.48	
BN-151	2.31	127	230	83	222	736	5	0.19	3D(4,4)-I; P4mbm[14]
BN-152	2.29	211	229	135	338	470	16	0.65	*scf*-B24N24[13]
BN-153	2.29	15	207	55	151	414	1	0.34	
BN-154	2.27	132	230	74	199	589	4	0.49	
BN-155	2.25	4	178	84	218	472	8	0.26	
BN-156	2.21	185	221	158	383	717	23	0.10	
BN-157	2.18	36	216	150	366	646	21	0.15	
BN-158	2.11	185	210	133	330	521	18	0.23	
BN-159	2.01	44	187	88	228	703	8	0.24	
BN-160	2.01	217	163	49	133	185	2	0.30	
BN-161	1.93	44	157	90	226	693	11	0.13	*lz2*-BN[22]
BN-162	1.81	186	171	69	184	561	5	0.23	
BN-163	1.79	4	93	56	141	507	9	0.19	
BN-164	1.73	156	90	31	82	263	1	0.56	
BN-165	1.53	38	103	61	152	553	9	0.11	
BN-166	1.32	217	123	35	96	229	1	0.75	
BN-167	1.29	174	127	28	79	406	-1	0.30	
BN-168	1.24	38	87	40	104	444	4	0.24	
BN-169	0.87	160	70	7	20	30	-3	1.29	
BN-170	0.84	136	61	6	18	23	-3	1.30	
BN-171	0.75	217	69	17	48	130	-1	0.82	

BN-172	3.88	215	392	332	776	1236	46	1.76	*Rocksalt*-BN[8,24-28] (thermodynamically unstable)
BN-173	3.41	10	363	351	797	933	56	0.10	3D(8,8)-I; P12m1[14]
BN-174	3.38	10	359	340	775	935	54	0.11	3D(6,6)-II; P12m1[14]
BN-175	3.38	45	357	353	796	1005	58	0.14	3D(12,0)-III; Iba2[14]
BN-176	3.36	10	346	336	762	872	55	0.37	*mP28*-BN[29]
BN-177	3.34	12	341	311	715	873	49	0.18	3D(6,6)-VI; C12m1[14]
BN-178	3.29	8	330	328	739	879	56	0.54	*M*-BN[1]
BN-179	3.27	36	312	289	663	831	47	0.22	M_2W_1[15]
BN-180	3.21	27	330	298	687	968	47	0.25	3D(10,0)-III; Pcc2[14]
BN-181	3.21	8	296	237	561	950	35	0.31	*M*-BN[15]
BN-182	2.99	108	243	207	484	856	35	0.35	3D(12,0)-II; I4cm[14]
BN-183	2.86	39	294	197	483	882	24	0.21	3D(10,0)-I; Abm2[14]
BN-184	2.79	65	253	153	382	896	18	0.15	3D(4,4)-V; Cmmm[14]
BN-185	2.73	10	255	146	369	800	16	0.23	3D(6,6)-V; P12m1[14]
BN-186	2.71	39	271	156	393	856	17	0.18	3D(12,0)-I; Abm2[14]
BN-187	2.56	84	232	144	358	860	18	0.18	3D(6,6)-I; P42m[14]
BN-188	2.50	105	255	148	372	774	17	0.25	3D(6,0)-I; P42mc[14]
BN-189	2.40	40	161	72	189	776	7	0.13	*dz4*-BN[22]
BN-190	2.40	1	150	104	253	874	17	0.01	B2N2(EQ1)[30]
BN-191	2.37	226	233	160	390	413	22	0.46	*sc*-$B_{12}N_{12}$[20]
BN-192	2.30	8	205	122	306	819	15	0.13	*IV*-BN[31]
BN-193	2.10	228	217	95	248	314	8	0.16	*d*-BN[1]
BN-194	1.86	187	186	55	149	494	2	0.45	P-6M2-BN[1]

Structural and mechanical information of mechanically stable BN structures

BN-001

Density (g/cm^3): 3.63 Space Group: 181
Bulk modulus (GPa): 382 Shear modulus (GPa): 364
Young's modulus (GPa): 829 Highest Young's modulus (GPa): 979
Hardness (GPa): 57 Energy above hull (eV/atom): 0.95

Primitive Cell

1.000000

2.60023571229346	0.00000000000000	0.00000000000000
-1.30011785614673	2.25187018267366	0.00000000000000
0.00000000000000	0.00000000000000	5.80979326602512

B N

3 3

DIRECT

0.5000000000000000	0.0000000000000000	0.0000000000000000
-0.0000000000000001	0.4999999999999999	0.3333333333333333
0.5000000000000000	0.4999999999999999	0.6666666666666665
0.5000000000000000	0.0000000000000000	0.5000000000000000
-0.0000000000000001	0.4999999999999999	0.8333333333333333
0.5000000000000000	0.4999999999999999	0.1666666666666665

Stiffness tensor (GPa):

870.516	152.910	98.880	-0.000	-0.003	-0.144
152.910	870.205	98.750	-0.001	0.011	-0.115
98.880	98.750	997.851	0.006	-0.003	-0.146
-0.000	-0.001	0.006	337.419	0.015	-0.007
-0.003	0.011	-0.003	0.015	337.245	-0.000
-0.144	-0.115	-0.146	-0.007	-0.000	358.912

BN-002

Density (g/cm^3): 3.63	Space Group: 5
Bulk modulus (GPa): 379	Shear modulus (GPa): 345
Young's modulus (GPa): 794	Highest Young's modulus (GPa): 981
Hardness (GPa): 52	Energy above hull (eV/atom): 1.01

Primitive Cell

1.000000

1.29367886393348	-2.25809975845922	0.00000000000000
1.29367886393348	2.25809975845922	0.00000000000000
-0.00002005655005	0.00000000000000	11.67396283319412

B N

6 6

DIRECT

0.0416766461872939	0.9583233538127061	0.0000000000000000
0.5416706838551875	0.4583293161448125	0.5000000000000000
0.5416693520476636	0.9583174277127062	0.8340489258292065
0.0416825722872938	0.4583306479523364	0.1659510741707935
0.5416806829645484	0.9583335189937952	0.3333271964814095
0.0416664810062047	0.4583193170354515	0.6666728035185905
0.0416664109040382	0.9583175332153165	0.7510666686553562
0.0416824667846835	0.9583335890959619	0.2489333313446438
0.0416734489100243	0.4583305120214358	0.4167073139808981
0.5416694879785642	0.9583265510899757	0.5832926860191019
0.0416733874890163	0.4583207370082385	0.9169444617675905
0.5416792629917615	0.9583266125109837	0.0830555382324095

Stiffness tensor (GPa):

881.142	150.628	88.779	0.031	0.152	-0.012
150.628	854.459	101.718	-0.027	0.159	-0.006
88.779	101.718	998.527	0.018	0.156	-0.007
0.031	-0.027	0.018	316.142	0.011	-0.001
0.152	0.159	0.156	0.011	288.598	-0.007
-0.012	-0.006	-0.007	-0.001	-0.007	339.759

BN-003

Density (g/cm^3): 3.63 | Space Group: 1

Bulk modulus (GPa): 379 | Shear modulus (GPa): 345

Young's modulus (GPa): 794 | Highest Young's modulus (GPa): 980

Hardness (GPa): 52 | Energy above hull (eV/atom): 1.01

Primitive Cell

1.000000

2.58730792668208	0.00000000000000	0.00000000000000
1.29365385268218	2.25842205071991	0.00000000000000
0.00003479701381	-0.00001033997695	11.67347952556202

B N

6 6

DIRECT

0.7499964568607107	0.5000054573337023	0.1662962178836754
0.7499843606222181	0.0000136699174291	0.4995665580150330
0.2500145308269284	0.4999815800963003	0.8336910258953751
0.2500058842737134	0.9999878554871851	0.9995666090512516
0.2499861448532454	0.5000175058301207	0.3336909613080511
0.7500060216731345	0.4999931136248021	0.6662962309093523
0.7499925227009212	0.0000116108114965	0.2507481523304106
0.2499993817478512	0.4999981851197191	0.0830092155326718
0.2499919939105771	0.5000037210219034	0.5830091938712847
0.7499851056506486	0.5000161962233366	0.4166814650676274
0.7500105635294813	0.4999839015177233	0.9166815307428793
0.2500126713505684	0.9999872910162692	0.7507481983923809

Stiffness tensor (GPa):

881.062	150.360	88.688	0.020	0.058	-0.017
150.360	854.470	102.050	-0.009	0.048	-0.015
88.688	102.050	997.892	0.007	0.060	-0.015
0.020	-0.009	0.007	315.341	0.012	0.013
0.058	0.048	0.060	0.012	288.355	-0.003
-0.017	-0.015	-0.015	0.013	-0.003	339.669

BN-004

Density (g/cm^3): 3.62 | Space Group: 21

Bulk modulus (GPa): 377 | Shear modulus (GPa): 330

Young's modulus (GPa): 765 | Highest Young's modulus (GPa): 982

Hardness (GPa): 48 | Energy above hull (eV/atom): 1.06

Primitive Cell

1.000000

1.28726305554560	-2.26464068902433	0.00000000000000
1.28726305554560	2.26464068902433	0.00000000000000
0.00000000000000	0.00000000000000	5.86311188131492

B N

3 3

DIRECT

0.0000000000000000	0.5000000000000000	0.8319308032964308
0.5000000000000000	0.0000000000000000	0.1680691967035693
0.5000000000000000	0.5000000000000000	0.4999999999999999
0.5000000000000000	0.0000000000000000	0.6660458412746573
0.0000000000000000	0.5000000000000000	0.3339541587253427
0.0000000000000000	0.0000000000000000	0.0000000000000000

Stiffness tensor (GPa):

891.897	147.522	78.353	-0.057	-0.025	-0.091
147.522	838.828	104.699	-0.021	-0.009	-0.087
78.353	104.699	999.499	-0.036	-0.030	-0.094
-0.057	-0.021	-0.036	296.638	0.019	-0.007
-0.025	-0.009	-0.030	0.019	260.527	0.000
-0.091	-0.087	-0.094	-0.007	0.000	317.916

BN-005

Density (g/cm^3): 3.60 | Space Group: 171
Bulk modulus (GPa): 372 | Shear modulus (GPa): 273
Young's modulus (GPa): 658 | Highest Young's modulus (GPa): 1001
Hardness (GPa): 34 | Energy above hull (eV/atom): 1.13

Primitive Cell

1.000000

2.58906419205662	0.00000000000000	0.00000000000000
-1.29453209602831	2.24219536234966	0.00000000000000
0.00000000000000	0.00000000000000	23.64040174638068

B N

12 12

DIRECT

0.5000000000000000	0.5000000000000000	0.5212645566915565
0.0000000000000000	0.5000000000000000	0.8545978900248898
0.5000000000000000	0.0000000000000000	0.1879312233582231
0.0000000000000000	0.0000000000000000	0.6043902452461061
0.0000000000000000	0.0000000000000000	0.9377235785794393
0.0000000000000000	0.0000000000000000	0.2710569119127726
0.5000000000000000	0.0000000000000000	0.7704100496938784
0.0000000000000000	0.5000000000000000	0.4370767163605449
0.5000000000000000	0.5000000000000000	0.1037433830272116
0.5000000000000000	0.5000000000000000	0.3539302310570371
0.0000000000000000	0.5000000000000000	0.6872635643903704
0.5000000000000000	0.0000000000000000	0.0205968977237037
0.5000000000000000	0.5000000000000000	0.8124541832386313
0.5000000000000000	0.0000000000000000	0.4791208499052979
0.0000000000000000	0.5000000000000000	0.1457875165719646
0.0000000000000000	0.0000000000000000	0.7284567680068295
0.0000000000000000	0.0000000000000000	0.3951234346734962
0.0000000000000000	0.0000000000000000	0.0617901013401627
0.0000000000000000	0.5000000000000000	0.5627797829232812
0.5000000000000000	0.0000000000000000	0.8961131162566145
0.5000000000000000	0.5000000000000000	0.2294464495899478
0.5000000000000000	0.5000000000000000	0.9796475161338474
0.5000000000000000	0.0000000000000000	0.6463141828005141
0.0000000000000000	0.5000000000000000	0.3129808494671806

Stiffness tensor (GPa):

825.748	178.795	81.775	0.018	0.007	-0.016
178.795	825.642	81.743	0.096	0.043	-0.028
81.775	81.743	1013.839	0.058	0.017	-0.018
0.018	0.096	0.058	178.484	-0.043	0.021
0.007	0.043	0.017	-0.043	177.962	-0.001
-0.016	-0.028	-0.018	0.021	-0.001	323.339

BN-006

Density (g/cm^3): 3.60 | Space Group: 43

Bulk modulus (GPa): 370 | Shear modulus (GPa): 322

Young's modulus (GPa): 749 | Highest Young's modulus (GPa): 958

Hardness (GPa): 47 | Energy above hull (eV/atom): 0.97

Primitive Cell

1.000000

0.00000000000000	2.13887145930935	7.75754761168338
1.38031413126449	0.00000000000000	7.75754761168338
1.38031413126449	2.13887145930935	0.00000000000000

B N

4 4

DIRECT

0.2809557738271922	0.2809557738271921	0.7190442261728078
0.5309557738271922	0.5309557738271922	0.9690442261728078
0.9068864684775964	0.9068864684775964	0.5931135315224036
0.6568864684775964	0.6568864684775964	0.3431135315224036
0.7191908512133155	0.7191908512133156	0.7808091487866844
0.4691908512133156	0.4691908512133155	0.5308091487866844
0.0929680291107687	0.0929680291107686	0.9070319708892314
0.3429680291107686	0.3429680291107686	0.1570319708892314

Stiffness tensor (GPa):

644.122	224.100	107.346	0.023	-0.083	-0.029
224.100	900.336	84.921	0.016	-0.046	-0.018
107.346	84.921	978.338	0.017	-0.063	-0.023
0.023	0.016	0.017	327.562	0.012	-0.007
-0.083	-0.046	-0.063	0.012	222.466	0.037
-0.029	-0.018	-0.023	-0.007	0.037	415.349

BN-007

Density (g/cm^3): 3.60 | Space Group: 21

Bulk modulus (GPa): 370 | Shear modulus (GPa): 265

Young's modulus (GPa): 641 | Highest Young's modulus (GPa): 1007

Hardness (GPa): 32 | Energy above hull (eV/atom): 1.18

Primitive Cell

1.000000

1.29283748420208	-2.23925853832019	0.00000000000000
1.29283748420208	2.23925853832019	0.00000000000000
0.00000000000000	0.00000000000000	17.81832686146997

B N

9 9

DIRECT

0.5000000000000000	0.0000000000000000	0.2782482085107378
0.0000000000000000	0.0000000000000000	0.6115816375888035
0.0000000000000000	0.5000000000000000	0.9449150423754888
0.5000000000000000	0.0000000000000000	0.0550849576245112
0.0000000000000000	0.5000000000000000	0.7217517914892622
0.0000000000000000	0.0000000000000000	0.3884183624111965
0.5000000000000000	0.5000000000000000	0.1666666155135985
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.8333333844864015
0.5000000000000000	0.0000000000000000	0.7776348975608187
0.0000000000000000	0.0000000000000000	0.1109680319467070
0.0000000000000000	0.5000000000000000	0.4443019783235718
0.5000000000000000	0.0000000000000000	0.5556980216764282
0.0000000000000000	0.5000000000000000	0.2223651024391813
0.0000000000000000	0.0000000000000000	0.8890319680532930
0.5000000000000000	0.5000000000000000	0.6666669674017813
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.3333330325982187

Stiffness tensor (GPa):

813.150	186.233	77.535	-0.069	0.102	-0.017
186.233	813.614	77.736	-0.099	0.037	-0.016
77.535	77.736	1019.348	-0.088	0.068	-0.022
-0.069	-0.099	-0.088	169.680	-0.021	0.055
0.102	0.037	0.068	-0.021	169.418	-0.016
-0.017	-0.016	-0.022	0.055	-0.016	313.463

BN-008

Density (g/cm^3): 3.55 | Space Group: 5
Bulk modulus (GPa): 354 | Shear modulus (GPa): 328
Young's modulus (GPa): 752 | Highest Young's modulus (GPa): 821
Hardness (GPa): 51 | Energy above hull (eV/atom): 0.99

Primitive Cell

1.000000

8.72395361052978	-1.30564700782570	0.00000000000000
8.72395361052978	1.30564700782570	0.00000000000000
-2.04307622959395	0.00000000000000	5.61010407456000

B N

11 11

DIRECT

0.5211748144738861	0.0737827282050285	0.1161233881523772
0.9262172717949715	0.4788251855261139	0.8838766118476228
0.6833105439387848	0.1800762497874389	0.5985897725183102
0.8199237502125611	0.3166894560612152	0.4014102274816898
0.1800760117847516	0.6833107466016433	0.2647973748435917
0.3166892533983567	0.8199239882152485	0.7352026251564083
0.0737824179211526	0.5211751956807176	0.4788348769972850
0.4788248043192824	0.9262175820788474	0.5211651230027150
0.9999999030603757	0.0000000969396243	0.0000000000000000
0.6381059783554022	0.6381060855212455	0.1381059529566701
0.3618939144787545	0.3618940216445978	0.8618940470433298
0.5490368480835667	0.0486847534363090	0.6311110097187032
0.9513152465636909	0.4509631519164334	0.3688889902812968
0.6812956774577307	0.1821885611254896	0.0985909870775311
0.8178114388745104	0.3187043225422693	0.9014090129224689
0.1821890949819379	0.6812952719085630	0.7648931419447721
0.3187047280914370	0.8178109050180622	0.2351068580552279
0.0486838100194293	0.5490377945455829	0.9666113933115793
0.4509622054544171	0.9513161899805707	0.0333886066884207
0.9999995714308927	0.0000004285691073	0.5000000000000000
0.6380749749601398	0.6380745704693211	0.6380740781638037
0.3619254295306788	0.3619250250398602	0.3619259218361964

Stiffness tensor (GPa):

797.453	104.042	134.949	-0.005	0.009	0.030
104.042	830.637	115.215	-0.015	0.003	0.052
134.949	115.215	855.797	-0.040	0.013	0.060
-0.005	-0.015	-0.040	280.678	-0.001	-0.004
0.009	0.003	0.013	-0.001	341.998	0.003
0.030	0.052	0.060	-0.004	0.003	315.237

BN-009

Density (g/cm^3): 3.54 | Space Group: 43

Bulk modulus (GPa): 334 | Shear modulus (GPa): 253

Young's modulus (GPa): 607 | Highest Young's modulus (GPa): 1175

Hardness (GPa): 34 | Energy above hull (eV/atom): 0.93

Primitive Cell

1.000000

0.00000000000000	2.47313003560072	3.87115089705130
1.21724554904263	0.00000000000000	3.87115089705130
1.21724554904263	2.47313003560072	0.00000000000000

B N

2 2

DIRECT

0.8121678964360737	0.8121678964360737	0.1878321035639263
0.0621678964360737	0.0621678964360737	0.4378321035639263
0.4378321002960019	0.4378321002960019	0.0621678997039981
0.1878321002960019	0.1878321002960019	0.8121678997039981

Stiffness tensor (GPa):

1178.673	30.555	52.916	0.035	0.063	-0.022
30.555	598.713	116.858	-0.032	0.004	-0.024
52.916	116.858	927.329	0.019	0.025	-0.021
0.035	-0.032	0.019	133.612	0.039	0.024
0.063	0.004	0.025	0.039	201.120	0.009
-0.022	-0.024	-0.021	0.024	0.009	230.511

BN-010

Density (g/cm^3): 3.53 | Space Group: 205

Bulk modulus (GPa): 333 | Shear modulus (GPa): 365

Young's modulus (GPa): 803 | Highest Young's modulus (GPa): 819

Hardness (GPa): 67 | Energy above hull (eV/atom): 0.64

Primitive Cell

1.000000

4.53722569926219	0.00000000000000	0.00000000000000
0.00000000000000	4.53722569926219	0.00000000000000
0.00000000000000	0.00000000000000	4.53722569926219

B N

8 8

DIRECT

0.8397568618288420	0.3397568618288420	0.1602431381711580
0.1602431381711580	0.6602431381711580	0.8397568618288420
0.3397568618288420	0.1602431381711580	0.8397568618288420
0.6602431381711580	0.8397568618288420	0.1602431381711580
0.1602431381711580	0.8397568618288420	0.3397568618288420
0.8397568618288420	0.1602431381711580	0.6602431381711580
0.6602431381711580	0.6602431381711580	0.6602431381711580
0.3397568618288420	0.3397568618288420	0.3397568618288420
0.1530295111419586	0.3469704888580414	0.6530295111419586
0.6530295111419586	0.3469704888580414	0.8469704888580414
0.3469704888580414	0.6530295111419586	0.1530295111419586
0.1530295111419586	0.1530295111419586	0.1530295111419586
0.8469704888580414	0.8469704888580414	0.8469704888580414
0.3469704888580414	0.8469704888580414	0.6530295111419586
0.6530295111419586	0.1530295111419586	0.3469704888580414
0.8469704888580414	0.6530295111419586	0.3469704888580414

Stiffness tensor (GPa):

834.007	83.180	83.141	0.036	0.016	-0.034
83.180	834.004	83.133	-0.019	0.010	0.012
83.141	83.133	834.005	0.029	0.025	0.027
0.036	-0.019	0.029	358.976	0.008	0.008
0.016	0.010	0.025	0.008	358.978	0.001
-0.034	0.012	0.027	0.008	0.001	358.961

BN-011

Density (g/cm^3): 3.53 | Space Group: 16

Bulk modulus (GPa): 331 | Shear modulus (GPa): 316

Young's modulus (GPa): 719 | Highest Young's modulus (GPa): 907

Hardness (GPa): 52 | Energy above hull (eV/atom): 0.95

Primitive Cell

1.000000

2.61784814691993	0.00000000000000	0.00000000000000
0.00000000000000	5.82746231943936	0.00000000000000
0.00000000000000	0.00000000000000	9.19277742503787

B N

12 12

DIRECT

0.5000000000000000	0.0000000000000000	0.2504101074829707
0.0000000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.7495898925170292
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.6592908212934738	0.6669360856514217	0.6261506170232579
0.2198495130196786	0.6657317437952892	0.8753637697863227
0.2198495130196786	0.3342682562047108	0.1246362302136773
0.6592908212934738	0.3330639143485783	0.3738493829767421
0.7801504869803213	0.6657317437952892	0.1246362302136773
0.3407091787065261	0.6669360856514217	0.3738493829767421
0.3407091787065261	0.3330639143485783	0.6261506170232579
0.7801504869803213	0.3342682562047108	0.8753637697863227
0.5000000000000000	0.4999999999999999	0.7542524104052093
0.0000000000000000	0.4999999999999999	0.0000000000000000
0.5000000000000000	0.4999999999999999	0.2457475895947907
0.5000000000000000	0.4999999999999999	0.5000000000000000
0.6980977954853309	0.1689085153172325	0.1250490260748127
0.2145959071587441	0.1666249185646023	0.3744804364154058
0.2145959071587441	0.8333750814353977	0.6255195635845942
0.6980977954853309	0.8310914846827675	0.8749509739251873
0.7854040928412558	0.1666249185646023	0.6255195635845942
0.3019022045146691	0.1689085153172325	0.8749509739251873
0.3019022045146691	0.8310914846827675	0.1250490260748127
0.7854040928412558	0.8333750814353977	0.3744804364154058

Stiffness tensor (GPa):

710.861	53.181	99.242	-0.018	0.013	-0.022
53.181	916.505	78.154	-0.025	0.003	0.017
99.242	78.154	908.610	-0.011	-0.006	0.026
-0.018	-0.025	-0.011	319.951	-0.014	0.007
0.013	0.003	-0.006	-0.014	262.964	-0.000
-0.022	0.017	0.026	0.007	-0.000	257.964

BN-012

Density (g/cm^3): 3.51 | Space Group: 20
Bulk modulus (GPa): 344 | Shear modulus (GPa): 315
Young's modulus (GPa): 723 | Highest Young's modulus (GPa): 813
Hardness (GPa): 49 | Energy above hull (eV/atom): 1.00

Primitive Cell

1.000000

3.02366399048138	-5.94109629050179	0.00000000000000
3.02366399048138	5.94109629050179	0.00000000000000
0.00000000000000	0.00000000000000	2.61417675192825

B N

8 8

DIRECT

0.1333486790100479	0.5024007512593379	0.9732648186812134
0.8666513209899521	0.4975992487406621	0.4732648186812134
0.6666080407840895	0.6666080407840895	0.0000000000000000
0.3333919592159104	0.3333919592159104	0.5000000000000000
0.4975992487406620	0.8666513209899520	0.5267351813187866
0.5024007512593380	0.1333486790100479	0.0267351813187866
0.9039568172028023	0.0960431827971977	0.7500000000000000
0.0960431827971977	0.9039568172028023	0.2500000000000000
0.6496642439761879	0.0151217288248520	0.9990944351616989
0.3503357560238121	0.9848782711751480	0.4990944351616990
0.1673269361313163	0.1673269361313163	0.0000000000000000
0.8326730638686837	0.8326730638686837	0.5000000000000000
0.9848782711751480	0.3503357560238121	0.5009055648383011
0.0151217288248520	0.6496642439761879	0.0009055648383011
0.4039809973948039	0.5960190026051961	0.7500000000000000
0.5960190026051961	0.4039809973948039	0.2500000000000000

Stiffness tensor (GPa):

768.759	123.729	102.984	-0.014	0.012	-0.021
123.729	849.861	128.930	0.003	0.012	-0.035
102.984	128.930	770.757	-0.021	-0.000	-0.022
-0.014	0.003	-0.021	333.807	0.006	-0.000
0.012	0.012	-0.000	0.006	307.949	-0.016
-0.021	-0.035	-0.022	-0.000	-0.016	261.632

BN-013

Density (g/cm^3): 3.50 | Space Group: 3
Bulk modulus (GPa): 291 | Shear modulus (GPa): 291
Young's modulus (GPa): 655 | Highest Young's modulus (GPa): 917
Hardness (GPa): 52 | Energy above hull (eV/atom): 1.00

Primitive Cell

1.000000

2.63075040841714	0.00000000000000	0.00000000000000
0.00000000000000	5.83729498147137	0.00000000000000
-1.31537758409292	0.00000000000000	6.89418577013988

B N

9 9

DIRECT

0.0000000000000000	0.8888871954694184	0.5000000000000001
0.1689404856645282	0.8888877167489644	0.8378794286869504
0.8310595143354718	0.8888877167489644	0.1621205713130495
0.9003434635578627	0.2253102040921741	0.6692516787881542
0.0996565364421373	0.2253102040921741	0.3307483212118459
0.5000000000000000	0.2230669551815910	0.0000000000000000
0.2689085143830593	0.5524645176031566	0.6692516669287207
0.7310914856169406	0.5524645176031566	0.3307483330712793
0.0000000000000000	0.5547092220792764	0.0000000000000000
0.0000000000000000	0.3888878775526972	0.5000000000000001
0.1704015604171402	0.3888885354507454	0.8408047799350159
0.8295984395828597	0.3888885354507454	0.1591952200649841
0.8524626089987613	0.7255392450621398	0.6681879706511680
0.1475373910012387	0.7255392450621398	0.3318120293488320
0.5000000000000000	0.7228017034030094	0.0000000000000000
0.3157279855180012	0.0522359521071358	0.6681880780512344
0.6842720144819987	0.0522359521071358	0.3318119219487656
0.0000000000000000	0.0549756349476804	0.0000000000000000

Stiffness tensor (GPa):

609.529	-13.335	79.673	0.010	-0.022	-0.046
-13.335	873.825	65.312	-0.004	-0.012	-0.005
79.673	65.312	932.155	-0.015	0.003	0.012
0.010	-0.004	-0.015	347.427	0.001	0.026
-0.022	-0.012	0.003	0.001	251.979	0.009
-0.046	-0.005	0.012	0.026	0.009	171.703

BN-014

Density (g/cm^3): 3.50 Space Group: 3

Bulk modulus (GPa): 319 Shear modulus (GPa): 304

Young's modulus (GPa): 692 Highest Young's modulus (GPa): 953

Hardness (GPa): 51 Energy above hull (eV/atom): 0.97

Primitive Cell

1.000000

4.63383126367458	0.00000000000000	0.00000000000000
0.00000000000000	2.62147130219907	0.00000000000000
-0.00000044660592	0.00000000000000	5.81082767179880

B N

6 6

DIRECT

0.7510244580571407	0.7910334398988335	0.3342642688958622
0.7510247892206100	0.1256307148552772	0.6657352644054402
0.2489752107793900	0.1256307148552772	0.3342647355945598
0.2489755419428593	0.7910334398988335	0.6657357311041379
0.5000000000000000	0.9583326781235241	0.0000000000000000
0.0000000000000000	0.4583325908809109	0.0000000000000000
0.2501739097841160	0.6802022168895145	0.1670011274903904
0.2501738826683679	0.2364663455318587	0.8329984379583986
0.7498261173316321	0.2364663455318587	0.1670015620416014
0.7498260902158840	0.6802022168895145	0.8329988725096096
-0.0000000000000000	0.9583340362645334	0.5000000000000000
0.5000000000000000	0.9583346876453704	0.5000000000000000

Stiffness tensor (GPa):

966.183	76.790	68.090	-0.005	-0.013	0.030
76.790	665.486	44.060	-0.016	-0.009	0.040
68.090	44.060	900.209	0.007	-0.016	0.033
-0.005	-0.016	0.007	238.515	0.006	0.018
-0.013	-0.009	-0.016	0.006	295.285	0.016
0.030	0.040	0.033	0.018	0.016	245.321

BN-015

Density (g/cm^3): 3.50 | Space Group: 5
Bulk modulus (GPa): 335 | Shear modulus (GPa): 313
Young's modulus (GPa): 715 | Highest Young's modulus (GPa): 913
Hardness (GPa): 50 | Energy above hull (eV/atom): 0.86

Primitive Cell

1.000000

6.27280961399608	-1.31560000321801	0.00000000000000
6.27280961399608	1.31560000321801	0.00000000000000
-3.61323039244167	0.00000000000000	6.42776661891168

B N

9 9

DIRECT

0.4829745035308803	0.5170254964691197	0.0000000000000000
0.8486655203111139	0.2073210339956297	0.7246563316392372
0.2383345125210301	0.0432718229930781	0.6133072549424980
0.9589571280136373	0.6471387620196989	0.9417578299939859
0.3528612379803011	0.0410428719863627	0.0582421700060141
0.9567281770069218	0.7616654874789699	0.3866927450575019
0.7926789660043703	0.1513344796888861	0.2753436683607628
0.6007792946174613	0.7305147268943734	0.3362369542767967
0.2694852731056268	0.3992207053825387	0.6637630457232033
0.9677618395938787	0.0322381604061213	0.5000000000000000
0.3255445696502798	0.7231587532410518	0.2234215441293363
0.7914300279972268	0.4927403029629663	0.1140590529772516
0.4377827923753614	0.1719219520818998	0.4424374808159972
0.8280780479181002	0.5622172076246387	0.5575625191840028
0.5072596970370338	0.2085699720027733	0.8859409470227484
0.2768412467589482	0.6744554303497202	0.7765784558706637
0.1006406376937270	0.2368035792666245	0.8391080191084955
0.7631964207333755	0.8993593623062730	0.1608919808915044

Stiffness tensor (GPa):

824.382	86.493	121.083	-0.017	-65.538	0.012
86.493	714.370	93.101	-0.002	-10.308	0.025
121.083	93.101	896.683	-0.023	44.349	0.036
-0.017	-0.002	-0.023	259.102	0.007	-37.838
-65.538	-10.308	44.349	0.007	363.458	-0.017
0.012	0.025	0.036	-37.838	-0.017	263.638

BN-016

Density (g/cm^3): 3.49 | Space Group: 33
Bulk modulus (GPa): 336 | Shear modulus (GPa): 310
Young's modulus (GPa): 711 | Highest Young's modulus (GPa): 1055
Hardness (GPa): 49 | Energy above hull (eV/atom): 0.72

Primitive Cell

1.000000

18.77189100091234	0.00000000000000	0.00000000000000
0.00000000000000	2.46492385330072	0.00000000000000
0.00000000000000	0.00000000000000	4.07975579675496

B N

16 16

DIRECT

0.3567227807886200	0.1644007083308787	0.5563358247847299
0.1432772192113800	0.6644007083308787	0.0563358247847299
0.6432772192113800	0.8355992916691213	0.0563358247847299
0.8567227807886200	0.3355992916691213	0.5563358247847299
0.2193643938761078	0.9762615550307974	0.6390456998868331
0.2806356061238922	0.4762615550307974	0.1390456998868332
0.7806356061238922	0.0237384449692026	0.1390456998868332
0.7193643938761078	0.5237384449692026	0.6390456998868331
0.5198436655779559	0.6244979775801820	0.0578900039306806
0.9801563344220441	0.1244979775801820	0.5578900039306806
0.4801563344220441	0.3755020224198180	0.5578900039306806
0.0198436655779559	0.8755020224198180	0.0578900039306806
0.6027929206121724	0.1450728049569268	0.5562676704791621
0.8972070793878276	0.6450728049569268	0.0562676704791620
0.3972070793878276	0.8549271950430732	0.0562676704791620
0.1027929206121723	0.3549271950430732	0.5562676704791621
0.1470131260253384	0.8428316524637143	0.4366539770373671
0.3529868739746616	0.3428316524637143	0.9366539770373671
0.8529868739746616	0.1571683475362857	0.9366539770373671
0.6470131260253384	0.6571683475362857	0.4366539770373671
0.2809081040644226	0.0126985099575012	0.3833214474943137
0.2190918959355774	0.5126985099575012	0.8833214474943136
0.7190918959355774	0.9873014900424988	0.8833214474943136
0.7809081040644226	0.4873014900424988	0.3833214474943137
0.9757702655095034	0.3773001657979123	0.9342617763649916
0.5242297344904966	0.8773001657979123	0.4342617763649916
0.0242297344904966	0.6226998342020877	0.4342617763649916
0.4757702655095035	0.1226998342020877	0.9342617763649916
0.9008419423947676	0.8501075182914994	0.4362235287591117
0.5991580576052324	0.3501075182914994	0.9362235287591116
0.0991580576052324	0.1498924817085006	0.9362235287591116
0.4008419423947676	0.6498924817085006	0.4362235287591117

Stiffness tensor (GPa):

719.406	34.490	153.041	0.056	0.046	-0.041
34.490	1058.982	50.593	0.009	0.022	0.020
153.041	50.593	789.980	0.001	0.035	0.008
0.056	0.009	0.001	277.687	0.013	0.007
0.046	0.022	0.035	0.013	305.705	0.013
-0.041	0.020	0.008	0.007	0.013	233.313

BN-017

Density (g/cm^3): 3.49 | Space Group: 216

Bulk modulus (GPa): 380 | Shear modulus (GPa): 390

Young's modulus (GPa): 871 | Highest Young's modulus (GPa): 974

Hardness (GPa): 65 | Energy above hull (eV/atom): 0.02

Primitive Cell

1.000000

0.00000000000000	1.80787151107102	1.80787151107102
1.80787151107102	0.00000000000000	1.80787151107102
1.80787151107102	1.80787151107102	0.00000000000000

B N

1 1

DIRECT

0.7500000000000000	0.7500000000000000	0.7500000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000

Stiffness tensor (GPa):

792.824	173.055	173.061	0.007	0.010	-0.003
173.055	792.799	173.045	-0.002	0.008	0.006
173.061	173.045	792.798	0.008	-0.001	0.010
0.007	-0.002	0.008	454.107	0.016	0.016
0.010	0.008	-0.001	0.016	454.100	0.003
-0.003	0.006	0.010	0.016	0.003	454.092

BN-018

Density (g/cm^3): 3.48 | Space Group: 186
Bulk modulus (GPa): 379 | Shear modulus (GPa): 390
Young's modulus (GPa): 871 | Highest Young's modulus (GPa): 1000
Hardness (GPa): 65 | Energy above hull (eV/atom): 0.03

Primitive Cell

```
  1.000000
    2.55229380041812    0.00000000000000    0.00000000000000
   -1.27614690020906    2.21035126908362    0.00000000000000
    0.00000000000000    0.00000000000000    8.38741478217332
  B     N
  4     4
DIRECT
    0.6666666666666666    0.3333333333333333    0.1559562465594626
    0.3333333333333333    0.6666666666666666    0.6559562465594626
    0.0000000000000000    0.0000000000000000    0.9066121028640339
    0.0000000000000000    0.0000000000000000    0.4066121028640339
    0.3333333333333333    0.6666666666666666    0.8441625027689438
    0.6666666666666667    0.3333333333333333    0.3441625027689436
    0.0000000000000000    0.0000000000000000    0.0932691483397494
    0.0000000000000000    0.0000000000000000    0.5932691483397494
```

Stiffness tensor (GPa):

934.684	134.970	66.565	0.015	-0.021	-0.005
134.970	934.553	66.534	0.006	-0.019	-0.007
66.565	66.534	1007.784	0.001	-0.022	0.039
0.015	0.006	0.001	346.374	0.007	0.015
-0.021	-0.019	-0.022	0.007	346.537	-0.013
-0.005	-0.007	0.039	0.015	-0.013	399.711

BN-019

Density (g/cm^3): 3.48 | Space Group: 160
Bulk modulus (GPa): 379 | Shear modulus (GPa): 390
Young's modulus (GPa): 870 | Highest Young's modulus (GPa): 999
Hardness (GPa): 65 | Energy above hull (eV/atom): 0.03

Primitive Cell

1.000000

1.27618039991012	0.73680309742263	8.38797652648534
-1.27618039991012	0.73680309742263	8.38797652648534
0.00000000000000	-1.47360619484526	8.38797652648534

B N

4 4

DIRECT

0.4065243208879699	0.4065243208879701	0.4065243208879701
0.2392837272949965	0.2392837272949965	0.2392837272949966
0.8229986376780990	0.8229986376780992	0.8229986376780992
0.6561374768182404	0.6561374768182405	0.6561374768182405
0.5934490769816749	0.5934490769816750	0.5934490769816749
0.7607452394155590	0.7607452394155593	0.7607452394155593
0.1770580025091135	0.1770580025091135	0.1770580025091136
0.3438035270399635	0.3438035270399636	0.3438035270399636

Stiffness tensor (GPa):

936.753	131.210	66.253	-33.496	-0.008	-0.020
131.210	936.693	66.233	33.470	-0.002	0.004
66.253	66.233	1006.839	-0.021	-0.007	0.017
-33.496	33.470	-0.021	346.319	-0.000	0.030
-0.008	-0.002	-0.007	-0.000	346.337	-33.452
-0.020	0.004	0.017	0.030	-33.452	402.658

BN-020

Density (g/cm^3): 3.48 | Space Group: 160

Bulk modulus (GPa): 378 | Shear modulus (GPa): 390

Young's modulus (GPa): 870 | Highest Young's modulus (GPa): 1007

Hardness (GPa): 65 | Energy above hull (eV/atom): 0.03

Primitive Cell

1.000000

1.27547370203404	0.73639508521364	6.30016766403408
-1.27547370203404	0.73639508521364	6.30016766403408
0.00000000000000	-1.47279017042729	6.30016766403408

B N

3 3

DIRECT

0.9585371971070766	0.9585371971070767	0.9585371971070767
0.1806707144744054	0.1806707144744055	0.1806707144744056
0.7358676352225281	0.7358676352225282	0.7358676352225282
0.0413856930947797	0.0413856930947798	0.0413856930947798
0.8193861602925061	0.8193861602925062	0.8193861602925062
0.2641525986698553	0.2641525986698554	0.2641525986698554

Stiffness tensor (GPa):

937.866	132.142	62.678	22.344	-0.001	-0.015
132.142	937.856	62.691	-22.308	-0.002	-0.008
62.678	62.691	1014.782	0.014	-0.000	0.016
22.344	-22.308	0.014	342.551	0.012	0.026
-0.001	-0.002	-0.000	0.012	342.526	22.309
-0.015	-0.008	0.016	0.026	22.309	402.462

BN-021

Density (g/cm^3): 3.48 | Space Group: 186

Bulk modulus (GPa): 379 | Shear modulus (GPa): 390

Young's modulus (GPa): 871 | Highest Young's modulus (GPa): 1025

Hardness (GPa): 65 | Energy above hull (eV/atom): 0.04

Primitive Cell

```
  1.000000
    2.54824981630378    0.00000000000000    0.00000000000000
   -1.27412490815189    2.20684907610810    0.00000000000000
    0.00000000000000    0.00000000000000    4.21302452997334
  B     N
  2     2
DIRECT
    0.3333333333333333  0.6666666666666666  0.0626907509287982
    0.6666666666666667  0.3333333333333333  0.5626907509287982
    0.6666666666666666  0.3333333333333333  0.9373092490675832
    0.3333333333333333  0.6666666666666666  0.4373092490675832
```

Stiffness tensor (GPa):

944.333	132.620	57.150	0.019	-0.024	-0.017
132.620	944.359	57.115	0.009	-0.011	-0.018
57.150	57.115	1031.288	0.003	-0.021	0.018
0.019	0.009	0.003	335.712	-0.000	0.001
-0.024	-0.011	-0.021	-0.000	335.781	-0.002
-0.017	-0.018	0.018	0.001	-0.002	405.783

BN-022

Density (g/cm^3): 3.47 | Space Group: 220

Bulk modulus (GPa): 365 | Shear modulus (GPa): 312

Young's modulus (GPa): 728 | Highest Young's modulus (GPa): 769

Hardness (GPa): 45 | Energy above hull (eV/atom): 0.73

Primitive Cell

1.000000

-2.61156223664050	2.61156223664050	2.61156223664050
2.61156223664050	-2.61156223664050	2.61156223664050
2.61156223664050	2.61156223664050	-2.61156223664050

B N

6 6

DIRECT

0.7500000000000000	0.3750000000000000	0.6250000000000000
0.2500000000000000	0.1250000000000000	0.8750000000000000
0.1250000000000000	0.8750000000000000	0.2500000000000000
0.3750000000000000	0.6250000000000000	0.7500000000000000
0.8750000000000000	0.2500000000000000	0.1250000000000000
0.6250000000000000	0.7500000000000000	0.3750000000000000
0.2500000000000000	0.6250000000000000	0.3750000000000000
0.7500000000000000	0.8750000000000000	0.1250000000000000
0.8750000000000000	0.1250000000000000	0.7500000000000000
0.6250000000000000	0.3750000000000000	0.2500000000000000
0.1250000000000000	0.7500000000000000	0.8750000000000000
0.3750000000000000	0.2500000000000000	0.6250000000000000

Stiffness tensor (GPa):

739.090	177.707	177.701	0.018	0.006	0.009
177.707	739.061	177.693	0.011	0.015	0.005
177.701	177.693	739.056	0.007	0.011	0.020
0.018	0.011	0.007	334.663	0.016	0.012
0.006	0.015	0.011	0.016	334.674	0.004
0.009	0.005	0.020	0.012	0.004	334.662

BN-023

Density (g/cm^3): 3.47 | Space Group: 29
Bulk modulus (GPa): 343 | Shear modulus (GPa): 290
Young's modulus (GPa): 679 | Highest Young's modulus (GPa): 938
Hardness (GPa): 42 | Energy above hull (eV/atom): 0.52

Primitive Cell

1.000000

9.05912496099722	0.00000000000000	0.00000000000000
0.00000000000000	2.49410999579978	0.00000000000000
0.00000000000000	0.00000000000000	8.41306300249431

B N

16 16

DIRECT

0.7097637133386727	0.1248030665022926	0.6548244284533161
0.2902362866613273	0.8751969334977074	0.1548244284533160
0.7902362866613273	0.1248030665022926	0.1548244284533160
0.2097637133386727	0.8751969334977074	0.6548244284533161
0.6340916097647563	0.8746383477702246	0.9076932247367656
0.3659083902352437	0.1253616522297754	0.4076932247367657
0.8659083902352437	0.8746383477702246	0.4076932247367657
0.1340916097647562	0.1253616522297754	0.9076932247367656
0.1169367749314447	0.4234554788486242	0.4053751903213480
0.8830632250685553	0.5765445211513758	0.9053751903213481
0.3830632250685553	0.4234554788486242	0.9053751903213481
0.6169367749314447	0.5765445211513758	0.4053751903213480
0.0378621169130344	0.6574014394727015	0.1575125794637253
0.9621378830869656	0.3425985605272985	0.6575125794637253
0.4621378830869656	0.6574014394727015	0.6575125794637253
0.5378621169130344	0.3425985605272985	0.1575125794637253
0.7805658206362555	0.3723023663360610	0.3452957454852717
0.2194341793637445	0.6276976336639390	0.8452957454852716
0.7194341793637445	0.3723023663360610	0.8452957454852716
0.2805658206362556	0.6276976336639390	0.3452957454852717
0.8777988944329760	0.6196759879199270	0.0913677405625038
0.1222011055670240	0.3803240120800730	0.5913677405625037
0.6222011055670240	0.6196759879199270	0.5913677405625037
0.3777988944329760	0.3803240120800730	0.0913677405625038
0.3720020509454844	0.1005487779188363	0.5941893807447790
0.6279979490545156	0.8994512220811637	0.0941893807447789
0.1279979490545156	0.1005487779188363	0.0941893807447789
0.8720020509454844	0.8994512220811637	0.5941893807447790
0.4729889179046727	0.8715352172631972	0.8437417464393607
0.5270110820953273	0.1284647827368028	0.3437417464393606
0.0270110820953273	0.8715352172631972	0.3437417464393606
0.9729889179046727	0.1284647827368028	0.8437417464393607

Stiffness tensor (GPa):

860.399	66.748	161.349	0.045	-0.004	-0.003
66.748	943.954	40.732	-0.032	0.055	0.014
161.349	40.732	755.393	-0.040	0.043	0.044
0.045	-0.032	-0.040	189.353	-0.002	0.037
-0.004	0.055	0.043	-0.002	297.494	0.008
-0.003	0.014	0.044	0.037	0.008	255.541

BN-024

Density (g/cm^3): 3.47 | Space Group: 39
Bulk modulus (GPa): 301 | Shear modulus (GPa): 255
Young's modulus (GPa): 597 | Highest Young's modulus (GPa): 785
Hardness (GPa): 39 | Energy above hull (eV/atom): 0.71

Primitive Cell

1.000000

2.47318009537749	0.00000000000000	0.00000000000000
0.00000000000000	7.49952966514065	3.84511042882130
0.00000000000000	-7.49952966514065	3.84511042882130

B N

12 12

DIRECT

0.7256473210792702	0.8555151441807969	0.0200280222631493
0.2743526789207298	0.3555151441807969	0.5200280222631493
0.2743526789207298	0.0200280222631493	0.8555151441807969
0.7256473210792702	0.5200280222631493	0.3555151441807969
0.5549226864278449	0.3496686765573662	0.0169269365475537
0.4450773135721551	0.8496686765573662	0.5169269365475537
0.4450773135721551	0.0169269365475537	0.3496686765573662
0.5549226864278449	0.5169269365475537	0.8496686765573662
0.0000000000000000	0.1874357111895995	0.1874357111895995
0.0000000000000000	0.6874357111895995	0.6874357111895995
0.9838604740099829	0.6874238892177797	0.1874238892177798
0.0161395259900171	0.1874238892177798	0.6874238892177797
0.7784454141842383	0.1449441765486432	0.9813269790521575
0.2215545858157618	0.6449441765486432	0.4813269790521574
0.2215545858157618	0.9813269790521575	0.1449441765486432
0.7784454141842383	0.4813269790521574	0.6449441765486432
0.9695104028928115	0.6496230963601894	0.9835275567696209
0.0304895971071885	0.1496230963601894	0.4835275567696209
0.0304895971071885	0.9835275567696209	0.6496230963601894
0.9695104028928115	0.4835275567696209	0.1496230963601894
0.4999999999999999	0.8116839739982233	0.8116839739982233
0.4999999999999999	0.3116839739982233	0.3116839739982233
0.5115844154293475	0.3118958194350667	0.8118958194350667
0.4884155845706525	0.8118958194350667	0.3118958194350667

Stiffness tensor (GPa):

757.515	117.027	-77.483	0.132	0.023	-0.001
117.027	649.640	192.468	0.030	0.057	-0.036
-77.483	192.468	853.636	0.087	0.034	-0.012
0.132	0.030	0.087	307.014	0.023	-0.070
0.023	0.057	0.034	0.023	216.949	0.007
-0.001	-0.036	-0.012	-0.070	0.007	155.252

BN-025

Density (g/cm^3): 3.46 Space Group: 33

Bulk modulus (GPa): 363 Shear modulus (GPa): 364

Young's modulus (GPa): 818 Highest Young's modulus (GPa): 924

Hardness (GPa): 60 Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

19.81230843606917	0.00000000000000	0.00000000000000
0.00000000000000	2.52467461019767	0.00000000000000
0.00000000000000	0.00000000000000	3.80669414123007

B N

16 16

DIRECT

0.1537471786361120	0.9900288862862618	0.8688718934278652
0.3462528213638880	0.4900288862862618	0.3688718934278652
0.8462528213638880	0.0099711137137382	0.3688718934278652
0.6537471786361120	0.5099711137137382	0.8688718934278652
0.7180759977288040	0.0115527845573198	0.3698176543054623
0.7819240022711960	0.5115527845573198	0.8698176543054623
0.2819240022711959	0.9884472154426802	0.8698176543054623
0.2180759977288040	0.4884472154426802	0.3698176543054623
0.0199313150224805	0.1696541760371122	0.9561007912821133
0.4800686849775195	0.6696541760371122	0.4561007912821133
0.9800686849775195	0.8303458239628878	0.4561007912821133
0.5199313150224805	0.3303458239628878	0.9561007912821133
0.9082850283247603	0.5368400069701842	0.8718010682950347
0.5917149716752397	0.0368400069701842	0.3718010682950346
0.0917149716752397	0.4631599930298158	0.3718010682950346
0.4082850283247603	0.9631599930298158	0.8718010682950347
0.3461309486736594	0.9894769478269865	0.1221947867767662
0.1538690513263405	0.4894769478269865	0.6221947867767662
0.6538690513263405	0.0105230521730135	0.6221947867767662
0.8461309486736595	0.5105230521730135	0.1221947867767662
0.7819001683272353	0.0120432556989547	0.6202611104844027
0.7180998316727647	0.5120432556989547	0.1202611104844027
0.2180998316727647	0.9879567443010453	0.1202611104844027
0.2819001683272352	0.4879567443010453	0.6202611104844027
0.4772427907047391	0.8282966933324110	0.0703743849475714
0.0227572092952608	0.3282966933324110	0.5703743849475714
0.5227572092952608	0.1717033066675890	0.5703743849475714
0.9772427907047392	0.6717033066675890	0.0703743849475714
0.5918833299651651	0.5001576750128400	0.1205782897968836
0.9081166700348349	0.0001576750128400	0.6205782897968836
0.4081166700348348	0.4998423249871600	0.6205782897968836
0.0918833299651651	0.9998423249871600	0.1205782897968836

Stiffness tensor (GPa):

895.586	31.227	159.529	0.020	0.009	0.014
31.227	936.231	100.509	0.034	0.026	0.013
159.529	100.509	853.760	0.053	0.036	0.008
0.020	0.034	0.053	373.776	0.004	-0.007
0.009	0.026	0.036	0.004	400.731	-0.007
0.014	0.013	0.008	-0.007	-0.007	271.243

BN-026

Density (g/cm^3): 3.45 | Space Group: 5

Bulk modulus (GPa): 354 | Shear modulus (GPa): 350

Young's modulus (GPa): 790 | Highest Young's modulus (GPa): 922

Hardness (GPa): 58 | Energy above hull (eV/atom): 0.37

Primitive Cell

1.000000

6.06721307422115	-1.95781204628481	0.00000000000000
6.06721307422115	1.95781204628481	0.00000000000000
-0.01177046603205	0.00000000000000	2.51252053592780

B N

5 5

DIRECT

0.6155791311967398	0.3844208688032602	0.5000000000000000
0.4838913031958190	0.0806715008114527	0.6730456287754610
0.9193284991885472	0.5161086968041810	0.3269543712245390
0.2198945631131554	0.9821264240495634	0.0306986785695540
0.0178735759504365	0.7801054368868447	0.9693013214304460
0.3718238002347942	0.6281761997652058	0.0000000000000000
0.5308431553952765	0.8955622199980003	0.1726468167770165
0.1044377800019996	0.4691568446047236	0.8273531832229835
0.7674229816957298	0.0310947912809857	0.5119730543590465
0.9689052087190142	0.2325770183042703	0.4880269456409535

Stiffness tensor (GPa):

874.823	151.043	44.729	0.011	-37.181	0.017
151.043	878.140	59.236	0.005	45.348	0.022
44.729	59.236	927.861	-0.000	4.651	0.031
0.011	0.005	-0.000	333.389	-0.008	48.975
-37.181	45.348	4.651	-0.008	268.090	-0.002
0.017	0.022	0.031	48.975	-0.002	378.976

BN-027

Density (g/cm^3): 3.45 | Space Group: 7

Bulk modulus (GPa): 322 | Shear modulus (GPa): 278

Young's modulus (GPa): 648 | Highest Young's modulus (GPa): 855

Hardness (GPa): 42 | Energy above hull (eV/atom): 0.74

Primitive Cell

1.000000

2.47322444880768	0.00000000000000	0.00000000000000
0.00000000000000	9.41769707132022	0.00000000000000
-2.26403379958934	0.00000000000000	4.10476575839554

B N

8 8

DIRECT

0.8493790554352034	0.8105775869904778	0.3596047442829177
0.8493790554352034	0.1894224130095222	0.8596047442829178
0.7962901273547112	0.3367179517595313	0.4440086463196090
0.7962901273547112	0.6632820482404687	0.9440086463196091
0.5840391670623242	0.4180502309637812	0.9467103848769568
0.5840391670623242	0.5819497690362188	0.4467103848769568
0.1476261851596818	0.0461692006042888	0.4354036898597345
0.1476261851596818	0.9538307993957112	0.9354036898597347
0.1334547967842773	0.1909521103622630	0.6171754863288590
0.1334547967842773	0.8090478896377370	0.1171754863288590
0.2116198943407257	0.6722987184119891	0.5663035648054313
0.2116198943407257	0.3277012815880109	0.0663035648054313
0.4333972816677380	0.5735558379146157	0.0692432178933354
0.4333972816677380	0.4264441620853843	0.5692432178933355
0.8441934634815391	0.9481176481754677	0.5615502409971893
0.8441934634815391	0.0518823518245323	0.0615502409971893

Stiffness tensor (GPa):

860.827	-15.697	101.649	0.020	-39.457	0.017
-15.697	775.737	156.360	0.012	7.869	0.109
101.649	156.360	790.072	0.007	-32.839	0.086
0.020	0.012	0.007	309.751	0.025	-28.467
-39.457	7.869	-32.839	0.025	244.504	-0.008
0.017	0.109	0.086	-28.467	-0.008	175.954

BN-028

Density (g/cm^3): 3.45 | Space Group: 152

Bulk modulus (GPa): 351 | Shear modulus (GPa): 346

Young's modulus (GPa): 782 | Highest Young's modulus (GPa): 1012

Hardness (GPa): 57 | Energy above hull (eV/atom): 0.57

Primitive Cell

1.000000

4.08416915483180	0.00000000000000	0.00000000000000
-2.04208457741590	3.53699424143716	0.00000000000000
0.00000000000000	0.00000000000000	2.48223121385938

B N

3 3

DIRECT

0.6108278160734630	0.0000000000000000	0.8333333333333333
0.0000000000000000	0.6108278160734630	0.1666666666666665
0.3891721839265370	0.3891721839265370	0.4999999999999999
0.3718511241452209	0.0000000000000000	0.3333333333333334
0.0000000000000000	0.3718511241452209	0.6666666666666665
0.6281488758547791	0.6281488758547791	0.0000000000000000

Stiffness tensor (GPa):

836.435	136.350	49.857	70.938	-0.006	-0.021
136.350	836.438	49.808	-70.950	-0.038	-0.029
49.857	49.808	1016.640	-0.049	-0.041	0.004
70.938	-70.950	-0.049	309.106	-0.016	-0.028
-0.006	-0.038	-0.041	-0.016	309.179	71.013
-0.021	-0.029	0.004	-0.028	71.013	350.422

BN-029

Density (g/cm^3): 3.45 | Space Group: 7

Bulk modulus (GPa): 357 | Shear modulus (GPa): 351

Young's modulus (GPa): 793 | Highest Young's modulus (GPa): 977

Hardness (GPa): 57 | Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

2.52800141177019	0.00000000000000	0.00000000000000
0.00000000000000	9.18583401104102	0.00000000000000
-2.26560140442319	0.00000000000000	4.11798497019207

B N

8 8

DIRECT

0.7900791922156143	0.7019316185286131	0.0592980921641867
0.7900791922156143	0.2980683814713869	0.5592980921641868
0.3160141913413542	0.5396314039354611	0.5624572615918182
0.3160141913413541	0.4603685960645389	0.0624572615918182
0.1576290167712189	0.0616852264534714	0.6354313560378755
0.1576290167712188	0.9383147735465286	0.1354313560378755
0.8506551253542214	0.2151827838948165	0.0574130244729915
0.8506551253542214	0.7848172161051835	0.5574130244729916
0.2120815979024026	0.3011331352104588	0.9369185181984705
0.2120815979024025	0.6988668647895413	0.4369185181984704
0.6851221105878755	0.4581550033099384	0.4367758467977673
0.6851221105878755	0.5418449966900616	0.9367758467977674
0.8388648494650153	0.9407824669350604	0.3760351046600582
0.8388648494650153	0.0592175330649396	0.8760351046600583
0.1495539066024403	0.7878085403932236	0.9356707952909966
0.1495539066024402	0.2121914596067764	0.4356707952909966

Stiffness tensor (GPa):

909.991	81.489	49.100	0.016	1.205	0.022
81.489	830.294	112.186	0.018	13.939	0.032
49.100	112.186	993.860	0.014	2.112	0.042
0.016	0.018	0.014	340.077	-0.001	16.662
1.205	13.939	2.112	-0.001	314.959	-0.014
0.022	0.032	0.042	16.662	-0.014	291.256

BN-030

Density (g/cm^3): 3.44 | Space Group: 55

Bulk modulus (GPa): 371 | Shear modulus (GPa): 370

Young's modulus (GPa): 833 | Highest Young's modulus (GPa): 937

Hardness (GPa): 60 | Energy above hull (eV/atom): 0.07

Primitive Cell

1.000000

4.24412439073592	0.00000000000000	0.00000000000000
0.00000000000000	17.69807695981349	0.00000000000000
0.00000000000000	0.00000000000000	2.54883126717838

B N

16 16

DIRECT

0.8277674180960422	0.2915767130338275	0.5000000000000000
0.3277674180960422	0.2084232869661724	0.5000000000000000
0.3287553988746259	0.4557301042169356	0.5000000000000000
0.8287553988746259	0.0442698957830643	0.5000000000000000
0.3281893914029799	0.3329991766073370	0.0000000000000000
0.8281893914029799	0.1670008233926629	0.0000000000000000
0.3286560185469538	0.0832794763754964	0.0000000000000000
0.8286560185469538	0.4167205236245036	0.0000000000000000
0.1722325819039578	0.7084232869661724	0.5000000000000000
0.6722325819039578	0.7915767130338276	0.5000000000000000
0.6712446011253741	0.5442698957830643	0.5000000000000000
0.1712446011253741	0.9557301042169357	0.5000000000000000
0.6718106085970201	0.6670008233926630	0.0000000000000000
0.1718106085970201	0.8329991766073370	0.0000000000000000
0.6713439814530462	0.9167205236245036	0.0000000000000000
0.1713439814530462	0.5832794763754965	0.0000000000000000
0.7025967458028902	0.2083244915231190	0.5000000000000000
0.2025967458028903	0.2916755084768809	0.5000000000000000
0.2013520851480783	0.0442151658848807	0.5000000000000000
0.7013520851480783	0.4557848341151192	0.5000000000000000
0.2027303043994988	0.1670140448060420	0.0000000000000000
0.7027303043994988	0.3329859551939578	0.0000000000000000
0.2003153356857696	0.4165755474870537	0.0000000000000000
0.7003153356857696	0.0834244525129462	0.0000000000000000
0.2974032541971098	0.7916755084768810	0.5000000000000000
0.7974032541971098	0.7083244915231190	0.5000000000000000
0.7986479148519217	0.9557848341151193	0.5000000000000000
0.2986479148519217	0.5442151658848808	0.5000000000000000
0.7972696956005012	0.8329859551939579	0.0000000000000000
0.2972696956005012	0.6670140448060422	0.0000000000000000
0.7996846643142304	0.5834244525129462	0.0000000000000000
0.2996846643142304	0.9165755474870538	0.0000000000000000

Stiffness tensor (GPa):

946.403	72.504	64.844	0.006	-0.012	-0.028
72.504	903.651	131.985	-0.005	0.010	-0.002
64.844	131.985	949.522	0.011	0.011	0.017
0.006	-0.005	0.011	390.832	0.025	0.004
-0.012	0.010	0.011	0.025	335.098	0.006
-0.028	-0.002	0.017	0.004	0.006	299.190

BN-031

Density (g/cm^3): 3.44 | Space Group: 33
Bulk modulus (GPa): 354 | Shear modulus (GPa): 338
Young's modulus (GPa): 768 | Highest Young's modulus (GPa): 950
Hardness (GPa): 54 | Energy above hull (eV/atom): 0.28

Primitive Cell

1.000000

18.38603141292518	0.00000000000000	0.00000000000000
0.00000000000000	2.52718897531372	0.00000000000000
0.00000000000000	0.00000000000000	4.12257118501293

B N

16 16

DIRECT

0.3581371284765758	0.7030479125618201	0.0578143013771158
0.1418628715234242	0.2030479125618201	0.5578143013771159
0.6418628715234242	0.2969520874381799	0.5578143013771159
0.8581371284765758	0.7969520874381799	0.0578143013771158
0.7189803011524991	0.0293907795951021	0.1345724526440381
0.7810196988475009	0.5293907795951021	0.6345724526440382
0.2810196988475009	0.9706092204048979	0.6345724526440382
0.2189803011524991	0.4706092204048979	0.1345724526440381
0.5196371699915748	0.7642729804521042	0.5605144863915216
0.9803628300084252	0.2642729804521042	0.0605144863915217
0.4803628300084252	0.2357270195478958	0.0605144863915217
0.0196371699915749	0.7357270195478958	0.5605144863915216
0.6009012929694035	0.7268458628616816	0.0581262054853115
0.8990987070305965	0.2268458628616816	0.5581262054853116
0.3990987070305965	0.2731541371383184	0.5581262054853116
0.1009012929694035	0.7731541371383184	0.0581262054853115
0.1433565669277859	0.2897841239549044	0.9356829639662653
0.3566434330722141	0.7897841239549044	0.4356829639662654
0.8566434330722141	0.7102158760450956	0.4356829639662654
0.6433565669277859	0.2102158760450956	0.9356829639662653
0.7798276084087306	0.9673177731192588	0.8820705023787205
0.7201723915912694	0.4673177731192588	0.3820705023787205
0.2201723915912694	0.0326822268807412	0.3820705023787205
0.2798276084087306	0.5326822268807412	0.8820705023787205
0.9793031416276383	0.2349705120039329	0.4351055011377635
0.5206968583723617	0.7349705120039329	0.9351055011377635
0.0206968583723617	0.7650294879960671	0.9351055011377635
0.4793031416276383	0.2650294879960671	0.4351055011377635
0.9005791508713460	0.2793497429611991	0.9361136210479566
0.5994208491286540	0.7793497429611991	0.4361136210479566
0.0994208491286540	0.7206502570388009	0.4361136210479566
0.4005791508713461	0.2206502570388009	0.9361136210479566

Stiffness tensor (GPa):

820.677	100.762	124.150	0.107	0.006	0.019
100.762	888.916	28.625	0.059	0.007	0.004
124.150	28.625	968.641	0.042	0.001	0.029
0.107	0.059	0.042	295.105	-0.002	0.007
0.006	0.007	0.001	-0.002	335.791	0.005
0.019	0.004	0.029	0.007	0.005	274.153

BN-032

Density (g/cm^3): 3.44 | Space Group: 4
Bulk modulus (GPa): 345 | Shear modulus (GPa): 342
Young's modulus (GPa): 771 | Highest Young's modulus (GPa): 929
Hardness (GPa): 57 | Energy above hull (eV/atom): 0.43

Primitive Cell

1.000000

2.50450091884388	0.00000000000000	0.00000000000000
0.00000000000000	3.98731767240655	0.00000000000000
-1.24853908207547	0.00000000000000	4.79869895765060

B N

4 4

DIRECT

0.7141165997608340	0.9486583704993857	0.0813071866295032
0.2858834002391660	0.4486583704993858	0.9186928133704968
0.1577424290025264	0.3658616398455973	0.3774380688456840
0.8422575709974736	0.8658616398455973	0.6225619311543160
0.8712210141101183	0.5652305907214916	0.0910455695518015
0.1287789858898817	0.0652305907214916	0.9089544304481985
0.7004186428629705	0.1202493875303907	0.3791077512611418
0.2995813571370295	0.6202493875303907	0.6208922487388582

Stiffness tensor (GPa):

932.784	41.438	40.774	0.002	4.446	0.014
41.438	870.892	140.320	-0.002	60.694	0.032
40.774	140.320	854.483	-0.002	-55.726	0.052
0.002	-0.002	-0.002	368.118	0.018	58.569
4.446	60.694	-55.726	0.018	261.399	0.010
0.014	0.032	0.052	58.569	0.010	319.266

BN-033

Density (g/cm^3): 3.44 | Space Group: 4
Bulk modulus (GPa): 350 | Shear modulus (GPa): 342
Young's modulus (GPa): 774 | Highest Young's modulus (GPa): 909
Hardness (GPa): 56 | Energy above hull (eV/atom): 0.31

Primitive Cell

1.000000

2.52283095435767	0.00000000000000	0.00000000000000
0.00000000000000	3.97497256634550	0.00000000000000
-0.00004662736543	0.00000000000000	9.55701129061951

B N

8 8

DIRECT

0.9673650050357641	0.5527606990972282	0.0790387936015258
0.0326349949642359	0.0527606990972282	0.9209612063984742
0.4431607449470384	0.5528669839243587	0.8422804481757096
0.5568392550529616	0.0528669839243587	0.1577195518242904
0.2883437817127715	0.6305572892891191	0.3062559685281858
0.7116562182872285	0.1305572892891191	0.6937440314718142
0.2530531736591267	0.6347895725303392	0.5668147833839543
0.7469468263408733	0.1347895725303392	0.4331852166160456
0.0405425253309063	0.9325088016384850	0.0746605596324454
0.9594574746690937	0.4325088016384850	0.9253394403675546
0.5474784842645817	0.9325642143636002	0.8381460040909943
0.4525215157354183	0.4325642143636002	0.1618539959090057
0.7309307782503511	0.8835733310757254	0.3076358822580678
0.2690692217496489	0.3835733310757254	0.6923641177419322
0.7517302376842727	0.8803791086011361	0.5673064039220779
0.2482697623157273	0.3803791086011361	0.4326935960779221

Stiffness tensor (GPa):

892.788	46.003	59.576	0.005	-2.328	0.024
46.003	936.715	126.744	0.007	-37.324	0.018
59.576	126.744	862.422	-0.020	35.419	0.098
0.005	0.007	-0.020	359.086	-0.003	-34.513
-2.328	-37.324	35.419	-0.003	251.679	0.009
0.024	0.018	0.098	-34.513	0.009	318.858

BN-034

Density (g/cm^3): 3.44 | Space Group: 33

Bulk modulus (GPa): 351 | Shear modulus (GPa): 342

Young's modulus (GPa): 775 | Highest Young's modulus (GPa): 909

Hardness (GPa): 56 | Energy above hull (eV/atom): 0.31

Primitive Cell

1.000000

19.11400299590764	0.00000000000000	0.00000000000000
0.00000000000000	2.52305641533058	0.00000000000000
0.00000000000000	0.00000000000000	3.97503573762556

B N

16 16

DIRECT

0.0788592392761465	0.4432139823727796	0.4471362621777422
0.5788592392761465	0.0567860176272203	0.4471362621777422
0.9211407607238535	0.5567860176272204	0.9471362621777423
0.4211407607238535	0.9432139823727796	0.9471362621777423
0.9604846719391917	0.9673947344936085	0.4472305879088209
0.4604846719391917	0.5326052655063915	0.4472305879088209
0.0395153280608083	0.0326052655063915	0.9472305879088210
0.5395153280608083	0.4673947344936084	0.9472305879088210
0.2833906268931642	0.7546962560727608	0.8652413265295010
0.7833906268931643	0.7453037439272392	0.8652413265295010
0.7166093731068357	0.2453037439272392	0.3652413265295009
0.2166093731068357	0.2546962560727608	0.3652413265295009
0.8468788191286747	0.2887983013137609	0.3695541332187312
0.3468788191286746	0.2112016986862390	0.3695541332187312
0.1531211808713253	0.7112016986862391	0.8695541332187313
0.6531211808713253	0.7887983013137609	0.8695541332187313
0.4190808016198870	0.0474458859557338	0.5674316562447492
0.9190808016198870	0.4525541140442661	0.5674316562447492
0.5809191983801130	0.9525541140442662	0.0674316562447492
0.0809191983801130	0.5474458859557338	0.0674316562447492
0.5373318467148449	0.5404805773099519	0.5674880513612597
0.0373318467148449	0.9595194226900481	0.5674880513612597
0.4626681532851550	0.4595194226900480	0.0674880513612597
0.9626681532851551	0.0404805773099519	0.0674880513612597
0.2163548718815253	0.7513440457408445	0.1195752012456430
0.7163548718815254	0.7486559542591555	0.1195752012456430
0.7836451281184746	0.2486559542591555	0.6195752012456430
0.2836451281184746	0.2513440457408444	0.6195752012456430
0.6538169967978751	0.2307151542663130	0.6163428232340034
0.1538169967978751	0.2692848457336869	0.6163428232340034
0.3461830032021249	0.7692848457336869	0.1163428232340031
0.8461830032021249	0.7307151542663131	0.1163428232340031

Stiffness tensor (GPa):

859.341	61.726	133.224	-0.046	0.005	0.017
61.726	890.508	44.573	-0.031	0.004	0.009
133.224	44.573	931.033	-0.013	-0.009	0.021
-0.046	-0.031	-0.013	315.595	0.001	0.012
0.005	0.004	-0.009	0.001	360.482	0.011
0.017	0.009	0.021	0.012	0.011	251.525

BN-035

Density (g/cm^3): 3.44 | Space Group: 31

Bulk modulus (GPa): 348 | Shear modulus (GPa): 338

Young's modulus (GPa): 767 | Highest Young's modulus (GPa): 916

Hardness (GPa): 55 | Energy above hull (eV/atom): 0.33

Primitive Cell

1.000000

16.57170667604314	0.00000000000000	0.00000000000000
0.00000000000000	2.52071384447360	0.00000000000000
0.00000000000000	0.00000000000000	4.01814920113991

B N

14 14

DIRECT

0.3407469985564702	0.9438346082683196	0.3040057602471363
0.1592530014435298	0.0561653917316804	0.8040057602471364
0.8407469985564702	0.0561653917316804	0.8040057602471364
0.6592530014435298	0.9438346082683196	0.3040057602471363
0.5735861756457312	0.2130930079910722	0.8824062781066928
0.9264138243542688	0.7869069920089278	0.3824062781066927
0.0735861756457312	0.7869069920089278	0.3824062781066927
0.4264138243542688	0.2130930079910722	0.8824062781066928
0.7043511093817798	0.5327794074680466	0.8044369826626248
0.7956488906182202	0.4672205925319534	0.3044369826626247
0.2043511093817798	0.4672205925319534	0.3044369826626247
0.2956488906182202	0.5327794074680466	0.8044369826626248
0.5000000000000000	0.7603229168543164	0.3854151904450182
0.0000000000000000	0.2396770831456835	0.8854151904450183
0.6565729686134171	0.0477883847216425	0.6832703509550093
0.8434270313865829	0.9522116152783575	0.1832703509550093
0.1565729686134172	0.9522116152783575	0.1832703509550093
0.3434270313865829	0.0477883847216425	0.6832703509550093
0.4268122505254930	0.7725444875290717	0.1350779892753874
0.0731877494745070	0.2274555124709283	0.6350779892753875
0.9268122505254930	0.2274555124709283	0.6350779892753875
0.5731877494745070	0.7725444875290717	0.1350779892753874
0.2928539631279943	0.4597123272736573	0.1832590592421904
0.2071460368720057	0.5402876727263427	0.6832590592421903
0.7928539631279943	0.5402876727263427	0.6832590592421903
0.7071460368720057	0.4597123272736573	0.1832590592421904
0.5000000000000000	0.2545822051455182	0.6296720791877017
0.0000000000000000	0.7454177948544818	0.1296720791877017

Stiffness tensor (GPa):

857.550	65.202	130.799	0.094	-0.001	0.045
65.202	883.400	31.798	0.044	0.011	0.041
130.799	31.798	936.992	0.005	-0.004	0.027
0.094	0.044	0.005	300.391	0.008	0.005

-0.001	0.011	-0.004	0.008	354.595	0.012
0.045	0.041	0.027	0.005	0.012	252.136

BN-036

Density (g/cm^3): 3.43 Space Group: 58

Bulk modulus (GPa): 368 Shear modulus (GPa): 364

Young's modulus (GPa): 821 Highest Young's modulus (GPa): 928

Hardness (GPa): 59 Energy above hull (eV/atom): 0.08

Primitive Cell

1.000000

4.25549290237676	0.00000000000000	0.00000000000000
0.00000000000000	13.28311938919532	0.00000000000000
0.00000000000000	0.00000000000000	2.54892383147475

B N

12 12

DIRECT

0.3284398662876122	0.3890763723615526	0.0000000000000000
0.8284398662876122	0.1109236276384476	0.4999999999999999
0.8276088205611163	0.2775190487969586	0.0000000000000000
0.3276088205611163	0.2224809512030415	0.4999999999999999
0.3286142955844134	0.0589467106327117	0.0000000000000000
0.8286142955844134	0.4410532893672884	0.4999999999999999
0.6715601337123878	0.6109236276384474	0.0000000000000000
0.1715601337123878	0.8890763723615525	0.4999999999999999
0.1723911794388837	0.7224809512030415	0.0000000000000000
0.6723911794388837	0.7775190487969585	0.4999999999999999
0.6713857044155866	0.9410532893672883	0.0000000000000000
0.1713857044155866	0.5589467106327116	0.4999999999999999
0.1999757698676341	0.1110290664058591	0.4999999999999999
0.6999757698676341	0.3889709335941410	0.0000000000000000
0.7024450287060341	0.2225632755819407	0.4999999999999999
0.2024450287060340	0.2774367244180594	0.0000000000000000
0.2009097185590698	0.4410257316451444	0.4999999999999999
0.7009097185590698	0.0589742683548558	0.0000000000000000
0.8000242301323659	0.8889709335941409	0.4999999999999999
0.3000242301323659	0.6110290664058590	0.0000000000000000
0.2975549712939659	0.7774367244180593	0.4999999999999999
0.7975549712939659	0.7225632755819407	0.0000000000000000
0.7990902814409302	0.5589742683548556	0.4999999999999999
0.2990902814409302	0.9410257316451442	0.0000000000000000

Stiffness tensor (GPa):

919.594	77.588	67.211	0.012	-0.012	-0.011
77.588	890.311	131.270	-0.007	0.010	-0.006
67.211	131.270	950.985	0.004	0.011	0.029
0.012	-0.007	0.004	386.210	0.019	0.006
-0.012	0.010	0.011	0.019	334.910	0.000
-0.011	-0.006	0.029	0.006	0.000	289.770

BN-037

Density (g/cm^3): 3.43 | Space Group: 26

Bulk modulus (GPa): 368 | Shear modulus (GPa): 364

Young's modulus (GPa): 822 | Highest Young's modulus (GPa): 928

Hardness (GPa): 59 | Energy above hull (eV/atom): 0.08

Primitive Cell

1.000000

2.54891050247347	0.00000000000000	0.00000000000000
0.00000000000000	13.28358138637460	0.00000000000000
0.00000000000000	0.00000000000000	4.25546113624656

B N

12 12

DIRECT

0.0000000000000000	0.8919937550478902	0.4167085200918874
0.0000000000000000	0.1080062449521098	0.9167085200918874
0.0000000000000000	0.2259481741027158	0.5737445774110201
0.0000000000000000	0.7740518258972842	0.0737445774110201
0.0000000000000000	0.5553649428998996	0.5724357773484740
0.0000000000000000	0.4446350571001004	0.0724357773484741
0.5000000000000000	0.0562181780521595	0.4163739280464770
0.5000000000000000	0.9437818219478405	0.9163739280464770
0.5000000000000000	0.7220631797792341	0.5732782669055796
0.5000000000000000	0.2779368202207659	0.0732782669055796
0.5000000000000000	0.3894153905201042	0.5728640469469672
0.5000000000000000	0.6105846094798958	0.0728640469469672
0.0000000000000000	0.1079443265615985	0.5441095937639489
0.0000000000000000	0.8920556734384015	0.0441095937639489
0.0000000000000000	0.7740317781143399	0.4458376815489540
0.0000000000000000	0.2259682218856601	0.9458376815489540
0.0000000000000000	0.4444509921110750	0.4472996760545087
0.0000000000000000	0.5555490078889250	0.9472996760545087
0.5000000000000000	0.9439868273724404	0.5449516627998083
0.5000000000000000	0.0560131726275596	0.0449516627998083
0.5000000000000000	0.2780314026666467	0.4449558096882518
0.5000000000000000	0.7219685973333533	0.9449558096882518
0.5000000000000000	0.6105071166641705	0.4474404592335497
0.5000000000000000	0.3894928833358295	0.9474404592335497

Stiffness tensor (GPa):

950.994	131.304	67.069	0.001	0.019	0.025
131.304	890.159	77.267	-0.007	0.022	0.019
67.069	77.267	919.798	-0.004	0.014	0.044
0.001	-0.007	-0.004	290.850	0.002	-0.001
0.019	0.022	0.014	0.002	335.048	0.004
0.025	0.019	0.044	-0.001	0.004	386.163

BN-038

Density (g/cm^3): 3.43 | Space Group: 29
Bulk modulus (GPa): 352 | Shear modulus (GPa): 345
Young's modulus (GPa): 780 | Highest Young's modulus (GPa): 854
Hardness (GPa): 57 | Energy above hull (eV/atom): 0.28

Primitive Cell

1.000000

4.87262360585908	0.00000000000000	0.00000000000000
0.00000000000000	4.42421773987862	0.00000000000000
0.00000000000000	0.00000000000000	8.91361371461369

B N

16 16

DIRECT

0.5156737933156507	0.5815602964825409	0.7663834472771168
0.4843262066843493	0.4184397035174591	0.2663834472771169
0.9843262066843493	0.5815602964825409	0.2663834472771169
0.0156737933156506	0.4184397035174591	0.7663834472771168
0.1840794018082874	0.0795012259648711	0.1360264579279713
0.8159205981917126	0.9204987740351289	0.6360264579279713
0.3159205981917126	0.0795012259648711	0.6360264579279713
0.6840794018082874	0.9204987740351289	0.1360264579279713
0.7136270706445100	0.4134482327488361	0.5176162310154152
0.2863729293554900	0.5865517672511639	0.0176162310154151
0.7863729293554900	0.4134482327488361	0.0176162310154151
0.2136270706445100	0.5865517672511639	0.5176162310154152
0.0548205121672518	0.0851029649842368	0.3894798353200809
0.9451794878327482	0.9148970350157632	0.8894798353200809
0.4451794878327482	0.0851029649842368	0.8894798353200809
0.5548205121672518	0.9148970350157632	0.3894798353200809
0.9831465097959463	0.9198729363717172	0.2328646532342208
0.0168534902040537	0.0801270636282828	0.7328646532342208
0.5168534902040537	0.9198729363717172	0.7328646532342208
0.4831465097959464	0.0801270636282828	0.2328646532342208
0.3143128867217113	0.4232782883475630	0.8653505344182971
0.6856871132782887	0.5767217116524370	0.3653505344182970
0.1856871132782887	0.4232782883475630	0.3653505344182970
0.8143128867217113	0.5767217116524370	0.8653505344182971
0.7840133827381406	0.0817760834706143	0.4819903655772010
0.2159866172618594	0.9182239165293857	0.9819903655772010
0.7159866172618594	0.0817760834706143	0.9819903655772010
0.2840133827381406	0.9182239165293857	0.4819903655772010
0.4439275130028755	0.4153198989102919	0.6102884944878935
0.5560724869971245	0.5846801010897081	0.1102884944878935
0.0560724869971245	0.4153198989102919	0.1102884944878935
0.9439275130028755	0.5846801010897081	0.6102884944878935

Stiffness tensor (GPa):

787.092	110.654	100.119	0.013	0.044	0.031
110.654	851.333	117.482	0.011	-0.004	0.022
100.119	117.482	876.160	0.009	0.027	0.037
0.013	0.011	0.009	383.691	0.003	0.002
0.044	-0.004	0.027	0.003	321.767	-0.003
0.031	0.022	0.037	0.002	-0.003	298.960

BN-039

Density (g/cm^3): 3.43 | Space Group: 31

Bulk modulus (GPa): 368 | Shear modulus (GPa): 364

Young's modulus (GPa): 821 | Highest Young's modulus (GPa): 929

Hardness (GPa): 59 | Energy above hull (eV/atom): 0.08

Primitive Cell

1.000000

2.54878898754823	0.00000000000000	0.00000000000000
0.00000000000000	13.27522527475752	0.00000000000000
0.00000000000000	0.00000000000000	4.25927429026245

B N

12 12

DIRECT

0.5000000000000000	0.1937332351881531	0.1821080537793157
0.0000000000000000	0.8062667648118469	0.6821080537793157
0.0000000000000000	0.6947524271409339	0.1820624620335920
0.5000000000000000	0.3052475728590661	0.6820624620335920
0.5000000000000000	0.5242072986954841	0.3395344197858399
0.0000000000000000	0.4757927013045159	0.8395344197858399
0.5000000000000000	0.8615834215099752	0.1827636922900436
0.0000000000000000	0.1384165784900248	0.6827636922900436
0.0000000000000000	0.0277316018010142	0.1823475661336337
0.5000000000000000	0.9722683981989858	0.6823475661336337
0.0000000000000000	0.3571273880507966	0.1802027542090291
0.5000000000000000	0.6428726119492034	0.6802027542090291
0.0000000000000000	0.8064180669111375	0.3075916199557187
0.5000000000000000	0.1935819330888625	0.8075916199557187
0.5000000000000000	0.3053252312567138	0.3101845597011765
0.0000000000000000	0.6946747687432862	0.8101845597011765
0.0000000000000000	0.4758962429929230	0.2080285249266501
0.5000000000000000	0.5241037570070770	0.7080285249266501
0.0000000000000000	0.1386582944638051	0.3077617711562486
0.5000000000000000	0.8613417055361949	0.8077617711562486
0.5000000000000000	0.9724828475922528	0.3077367644034018
0.0000000000000000	0.0275171524077472	0.8077367644034018
0.5000000000000000	0.6429495419291634	0.3096778088644324
0.0000000000000000	0.3570504580708366	0.8096778088644324

Stiffness tensor (GPa):

951.449	130.051	68.733	0.012	-0.019	0.025
130.051	883.814	84.496	-0.006	-0.019	0.018
68.733	84.496	909.074	0.012	-0.027	0.056
0.012	-0.006	0.012	295.172	0.002	0.010
-0.019	-0.019	-0.027	0.002	335.291	0.003
0.025	0.018	0.056	0.010	0.003	384.678

BN-040

Density (g/cm^3): 3.43 | Space Group: 8
Bulk modulus (GPa): 344 | Shear modulus (GPa): 342
Young's modulus (GPa): 770 | Highest Young's modulus (GPa): 944
Hardness (GPa): 57 | Energy above hull (eV/atom): 0.32

Primitive Cell

1.000000

2.01509176089122	-8.29214445407691	0.00000000000000
2.01509176089122	8.29214445407691	0.00000000000000
-0.17890247926527	0.00000000000000	2.51795042543496

B N

7 7

DIRECT

0.1466808632672771	0.4637550698904240	0.4549072746237727
0.4637550698904240	0.1466808632672771	0.4549072746237727
0.9569218535027346	0.8100672581914842	0.7200024845237760
0.8100672581914843	0.9569218535027346	0.7200024845237760
0.0116736655340690	0.6025280809868903	0.0116948009387220
0.6025280809868903	0.0116736655340690	0.0116948009387220
0.3815121185866230	0.3815121185866231	0.2698733319765334
0.8401959525488076	0.5283976012967584	0.5344292298409635
0.5283976012967584	0.8401959525488076	0.5344292298409635
0.0564927406973538	0.2026396448601886	0.2823556917477881
0.2026396448601887	0.0564927406973538	0.2823556917477881
0.9779370017673392	0.3926435309130498	0.9803650949905225
0.3926435309130498	0.9779370017673392	0.9803650949905225
0.6285546153819310	0.6285546153819310	0.7626173966512888

Stiffness tensor (GPa):

952.137	124.459	49.849	0.015	41.513	0.018
124.459	852.516	40.777	0.003	-0.811	0.011
49.849	40.777	870.386	0.033	1.522	0.045
0.015	0.003	0.033	254.226	-0.003	6.460
41.513	-0.811	1.522	-0.003	312.639	0.004
0.018	0.011	0.045	6.460	0.004	354.209

BN-041

Density (g/cm^3): 3.43 | Space Group: 4

Bulk modulus (GPa): 334 | Shear modulus (GPa): 329

Young's modulus (GPa): 744 | Highest Young's modulus (GPa): 892

Hardness (GPa): 55 | Energy above hull (eV/atom): 0.35

Primitive Cell

1.000000

2.51967230620670	0.00000000000000	0.00000000000000
0.00000000000000	4.08103951278834	0.00000000000000
-0.05297879081979	0.00000000000000	7.01737832959306

B N

6 6

DIRECT

0.4420231544031552	0.0568543816759635	0.7859414353659497
0.5579768455968448	0.5568543816759635	0.2140585646340502
0.0297726927127090	0.5571281194391202	0.8929459680763671
0.9702273072872909	0.0571281194391202	0.1070540319236329
0.7047805191579394	0.6333517432326663	0.5832970332211913
0.2952194808420606	0.1333517432326663	0.4167029667788087
0.5414777709742086	0.4351653748853508	0.7815374000917386
0.4585222290257914	0.9351653748853509	0.2184625999082614
0.9592244117110350	0.9350124236804725	0.8976947585289360
0.0407755882889650	0.4350124236804724	0.1023052414710640
0.2680372824399548	0.8824879603068814	0.5804856475124782
0.7319627175600452	0.3824879603068813	0.4195143524875217

Stiffness tensor (GPa):

848.920	0.910	76.629	0.050	2.522	-0.034
0.910	922.743	120.866	0.035	-51.029	-0.027
76.629	120.866	845.952	0.041	58.535	-0.020
0.050	0.035	0.041	346.701	0.009	-43.020
2.522	-51.029	58.535	0.009	251.323	0.001
-0.034	-0.027	-0.020	-43.020	0.001	291.455

BN-042

Density (g/cm^3): 3.42 | Space Group: 33
Bulk modulus (GPa): 289 | Shear modulus (GPa): 310
Young's modulus (GPa): 685 | Highest Young's modulus (GPa): 816
Hardness (GPa): 59 | Energy above hull (eV/atom): 0.29

Primitive Cell

1.000000

18.44480160691620	0.00000000000000	0.00000000000000
0.00000000000000	2.53191636966815	0.00000000000000
0.00000000000000	0.00000000000000	4.12386620428967

B N

16 16

DIRECT

0.6083700492500700	0.9382082879018145	0.4421497408307710
0.1083700492500701	0.5617917120981853	0.4421497408307710
0.3916299507499300	0.0617917120981855	0.9421497408307711
0.8916299507499300	0.4382082879018147	0.9421497408307711
0.4682138676185416	0.8105519450003411	0.3700126273102591
0.9682138676185417	0.6894480549996589	0.3700126273102591
0.5317861323814583	0.1894480549996589	0.8700126273102591
0.0317861323814584	0.3105519450003412	0.8700126273102591
0.7696373565061507	0.9781835993157674	0.9393222232033389
0.2696373565061507	0.5218164006842325	0.9393222232033389
0.2303626434938493	0.0218164006842326	0.4393222232033389
0.7303626434938493	0.4781835993157674	0.4393222232033389
0.8505164506165774	0.0023275199202657	0.4412624515452006
0.3505164506165774	0.4976724800797344	0.4412624515452006
0.1494835493834226	0.9976724800797343	0.9412624515452006
0.6494835493834226	0.5023275199202656	0.9412624515452006
0.8929076103413377	0.5211398666388277	0.5642042283910923
0.3929076103413376	0.9788601333611722	0.5642042283910923
0.1070923896586623	0.4788601333611723	0.0642042283910924
0.6070923896586623	0.0211398666388278	0.0642042283910924
0.0304702157197923	0.7273480831707650	0.6146933466204126
0.5304702157197924	0.7726519168292347	0.6146933466204126
0.9695297842802076	0.2726519168292349	0.1146933466204128
0.4695297842802077	0.2273480831707651	0.1146933466204128
0.7293489307900172	0.4863945532988844	0.0646472574617448
0.2293489307900172	0.0136054467011157	0.0646472574617448
0.2706510692099828	0.5136054467011156	0.5646472574617448
0.7706510692099828	0.9863945532988843	0.5646472574617448
0.6508713751044100	0.4589757313311417	0.5637082482141518
0.1508713751044100	0.0410242686688585	0.5637082482141518
0.3491286248955900	0.5410242686688583	0.0637082482141518
0.8491286248955900	0.9589757313311416	0.0637082482141518

Stiffness tensor (GPa):

839.732	139.751	159.540	-0.081	-0.002	0.038
139.751	657.614	-124.927	-0.382	0.001	-0.014
159.540	-124.927	847.622	-0.232	0.017	0.019
-0.081	-0.382	-0.232	264.503	0.013	-0.003
-0.002	0.001	0.017	0.013	343.900	-0.001
0.038	-0.014	0.019	-0.003	-0.001	261.492

BN-043

Density (g/cm^3): 3.42 | Space Group: 29

Bulk modulus (GPa): 341 | Shear modulus (GPa): 323

Young's modulus (GPa): 736 | Highest Young's modulus (GPa): 867

Hardness (GPa): 52 | Energy above hull (eV/atom): 0.40

Primitive Cell

1.000000

4.81724640382075	0.00000000000000	0.00000000000000
0.00000000000000	4.47840419197983	0.00000000000000
0.00000000000000	0.00000000000000	4.46997620745304

B N

8 8

DIRECT

0.3336405028951224	0.4217116103454698	0.5249298872993231
0.6663594971048776	0.5782883896545301	0.0249298872993231
0.1663594971048775	0.4217116103454698	0.0249298872993231
0.8336405028951225	0.5782883896545301	0.5249298872993231
0.8810408004989259	0.0839946326020708	0.2864159633067742
0.1189591995010741	0.9160053673979291	0.7864159633067742
0.6189591995010741	0.0839946326020708	0.7864159633067742
0.3810408004989258	0.9160053673979291	0.2864159633067742
0.1648432084154687	0.0747662268449882	0.4763391935139135
0.8351567915845313	0.9252337731550118	0.9763391935139135
0.3351567915845312	0.0747662268449882	0.9763391935139135
0.6648432084154687	0.9252337731550118	0.4763391935139135
0.6188701354540671	0.4220365860084735	0.7123149485254072
0.3811298645459330	0.5779634139915264	0.2123149485254072
0.8811298645459330	0.4220365860084735	0.2123149485254072
0.1188701354540669	0.5779634139915264	0.7123149485254072

Stiffness tensor (GPa):

696.082	82.826	142.006	0.013	0.043	-0.018
82.826	792.789	124.088	-0.008	-0.011	0.011
142.006	124.088	906.833	-0.005	-0.014	0.019
0.013	-0.008	-0.005	361.892	0.004	0.027
0.043	-0.011	-0.014	0.004	375.244	0.016
-0.018	0.011	0.019	0.027	0.016	225.993

BN-044

Density (g/cm^3): 3.41 | Space Group: 55

Bulk modulus (GPa): 362 | Shear modulus (GPa): 353

Young's modulus (GPa): 800 | Highest Young's modulus (GPa): 931

Hardness (GPa): 57 | Energy above hull (eV/atom): 0.10

Primitive Cell

1.000000

4.27989821898234	0.00000000000000	0.00000000000000
0.00000000000000	8.86752886786148	0.00000000000000
0.00000000000000	0.00000000000000	2.54894016647035

B N

8 8

DIRECT

0.8277422430423437	0.3340476885841671	0.0000000000000000
0.3277422430423437	0.1659523114158329	0.0000000000000000
0.8280087503437921	0.0882112013714278	0.5000000000000000
0.3280087503437920	0.4117887986285723	0.5000000000000000
0.1722577569576563	0.6659523114158330	0.0000000000000000
0.6722577569576564	0.8340476885841670	0.0000000000000000
0.1719912496562079	0.9117887986285722	0.5000000000000000
0.6719912496562079	0.5882112013714278	0.5000000000000000
0.6991992003883341	0.1658503740999903	0.0000000000000000
0.1991992003883340	0.3341496259000096	0.0000000000000000
0.6997791080980307	0.4113187759189221	0.5000000000000000
0.1997791080980306	0.0886812240810779	0.5000000000000000
0.3008007996116659	0.8341496259000096	0.0000000000000000
0.8008007996116659	0.6658503740999904	0.0000000000000000
0.3002208919019693	0.5886812240810779	0.5000000000000000
0.8002208919019693	0.9113187759189221	0.5000000000000000

Stiffness tensor (GPa):

869.179	87.081	71.563	-0.012	0.001	-0.015
87.081	864.636	130.555	-0.002	0.016	0.000
71.563	130.555	955.041	0.006	0.018	0.005
-0.012	-0.002	0.006	376.396	0.017	-0.013
0.001	0.016	0.018	0.017	334.848	0.006
-0.015	0.000	0.005	-0.013	0.006	274.401

BN-045

Density (g/cm^3): 3.41 | Space Group: 14

Bulk modulus (GPa): 344 | Shear modulus (GPa): 328

Young's modulus (GPa): 746 | Highest Young's modulus (GPa): 936

Hardness (GPa): 53 | Energy above hull (eV/atom): 0.36

Primitive Cell

1.000000

2.52032683073424	0.00000000000000	0.00000000000000
0.00000000000000	14.02237297078783	0.00000000000000
-2.20161043977912	0.00000000000000	4.10601820042850

B N

12 12

DIRECT

0.2975633424581412	0.9426704884113193	0.8277685732517606
0.7024366575418588	0.0573295115886807	0.1722314267482394
0.7024366575418588	0.4426704884113192	0.6722314267482394
0.2975633424581412	0.5573295115886807	0.3277685732517605
0.6813867465634018	0.7899033406688685	0.9074260454672403
0.3186132534365982	0.2100966593311315	0.0925739545327597
0.3186132534365982	0.2899033406688684	0.5925739545327597
0.6813867465634018	0.7100966593311315	0.4074260454672402
0.3793501576132869	0.8927083764204787	0.3278872954656193
0.6206498423867131	0.1072916235795213	0.6721127045343807
0.6206498423867131	0.3927083764204786	0.1721127045343806
0.3793501576132869	0.6072916235795214	0.8278872954656193
0.7517656703407594	0.9463890621035473	0.2080426716250414
0.2482343296592406	0.0536109378964527	0.7919573283749586
0.2482343296592406	0.4463890621035473	0.2919573283749585
0.7517656703407594	0.5536109378964527	0.7080426716250414
0.3638073675828821	0.7890024457133564	0.1454383127548349
0.6361926324171179	0.2109975542866435	0.8545616872451651
0.6361926324171179	0.2890024457133564	0.3545616872451650
0.3638073675828821	0.7109975542866436	0.6454383127548349
0.6675903479020658	0.8891070507537410	0.7043583148068608
0.3324096520979342	0.1108929492462590	0.2956416851931391
0.3324096520979342	0.3891070507537408	0.7956416851931392
0.6675903479020658	0.6108929492462591	0.2043583148068608

Stiffness tensor (GPa):

945.479	73.099	59.834	0.021	7.511	0.026
73.099	780.445	117.765	-0.013	26.715	0.047
59.834	117.765	873.963	0.018	-4.172	0.041
0.021	-0.013	0.018	297.785	0.012	18.541
7.511	26.715	-4.172	0.012	312.850	-0.019
0.026	0.047	0.041	18.541	-0.019	269.328

BN-046

Density (g/cm^3): 3.41 | Space Group: 31
Bulk modulus (GPa): 363 | Shear modulus (GPa): 352
Young's modulus (GPa): 797 | Highest Young's modulus (GPa): 932
Hardness (GPa): 57 | Energy above hull (eV/atom): 0.10

Primitive Cell

1.000000

2.54869253667817	0.00000000000000	0.00000000000000
0.00000000000000	8.85784691718253	0.00000000000000
0.00000000000000	0.00000000000000	4.28638099612044

B N

8 8

DIRECT

0.5000000000000000	0.5363643158824130	0.3361968370363667
0.0000000000000000	0.4636356841175870	0.8361968370363667
0.5000000000000000	0.2083065738982553	0.6799456049500010
0.0000000000000000	0.7916934261017446	0.1799456049500010
0.5000000000000000	0.7137656117087603	0.6777244991615233
0.0000000000000000	0.2862343882912396	0.1777244991615232
0.5000000000000000	0.0414386388294685	0.1805873693980879
0.0000000000000000	0.9585613611705315	0.6805873693980879
0.0000000000000000	0.4643277928249545	0.2038260421621301
0.5000000000000000	0.5356722071750455	0.7038260421621301
0.0000000000000000	0.7911287099212468	0.8082098804954170
0.5000000000000000	0.2088712900787531	0.3082098804954170
0.0000000000000000	0.2856591294985923	0.8079671947042768
0.5000000000000000	0.7143408705014076	0.3079671947042768
0.0000000000000000	0.9592172638577923	0.3055425714273015
0.5000000000000000	0.0407827361422077	0.8055425714273015

Stiffness tensor (GPa):

956.035	128.440	74.955	0.004	0.018	-0.001
128.440	855.492	98.952	-0.001	0.020	-0.006
74.955	98.952	853.937	-0.002	0.001	-0.008
0.004	-0.001	-0.002	278.359	0.009	0.003
0.018	0.020	0.001	0.009	334.813	0.009
-0.001	-0.006	-0.008	0.003	0.009	374.217

BN-047

Density (g/cm^3): 3.41 | Space Group: 61
Bulk modulus (GPa): 363 | Shear modulus (GPa): 354
Young's modulus (GPa): 801 | Highest Young's modulus (GPa): 896
Hardness (GPa): 57 | Energy above hull (eV/atom): 0.10

Primitive Cell

1.000000

4.28030182357802	0.00000000000000	0.00000000000000
0.00000000000000	10.23003530850217	0.00000000000000
0.00000000000000	0.00000000000000	4.41953182581041

B N

16 16

DIRECT

0.3295202937124502	0.0664009048306464	0.5882684317012512
0.8295202937124502	0.0664009048306464	0.9117315682987488
0.3295202937124502	0.4335990951693535	0.0882684317012512
0.8295202937124502	0.4335990951693535	0.4117315682987487
0.3275070093202713	0.1873081565935150	0.0835296346424761
0.8275070093202713	0.1873081565935150	0.4164703653575239
0.3275070093202713	0.3126918434064849	0.5835296346424761
0.8275070093202713	0.3126918434064849	0.9164703653575239
0.6704797062875498	0.9335990951693536	0.4117315682987487
0.1704797062875498	0.9335990951693536	0.0882684317012512
0.6704797062875498	0.5664009048306465	0.9117315682987488
0.1704797062875498	0.5664009048306465	0.5882684317012512
0.6724929906797287	0.8126918434064849	0.9164703653575239
0.1724929906797287	0.8126918434064849	0.5835296346424761
0.6724929906797287	0.6873081565935151	0.4164703653575239
0.1724929906797287	0.6873081565935151	0.0835296346424761
0.1993562697046104	0.4335068889570776	0.4118937048178316
0.6993562697046104	0.4335068889570776	0.0881062951821684
0.1993562697046104	0.0664931110429223	0.9118937048178316
0.6993562697046104	0.0664931110429223	0.5881062951821685
0.2009206811160922	0.3127355750028908	0.9153585143338073
0.7009206811160922	0.3127355750028908	0.5846414856661928
0.2009206811160922	0.1872644249971091	0.4153585143338074
0.7009206811160922	0.1872644249971091	0.0846414856661927
0.8006437302953896	0.5664931110429224	0.5881062951821685
0.3006437302953896	0.5664931110429224	0.9118937048178316
0.8006437302953896	0.9335068889570777	0.0881062951821684
0.3006437302953896	0.9335068889570777	0.4118937048178316
0.7990793188839078	0.6872644249971092	0.0846414856661927
0.2990793188839078	0.6872644249971092	0.4153585143338074
0.7990793188839078	0.8127355750028908	0.5846414856661928
0.2990793188839078	0.8127355750028908	0.9153585143338073

Stiffness tensor (GPa):

862.098	85.350	75.637	0.004	-0.011	-0.006
85.350	881.500	139.459	0.002	0.016	0.005
75.637	139.459	922.399	-0.003	0.010	0.020
0.004	0.002	-0.003	385.574	0.001	0.001
-0.011	0.016	0.010	0.001	321.426	0.003
-0.006	0.005	0.020	0.001	0.003	290.125

BN-048

Density (g/cm^3): 3.38 | Space Group: 186
Bulk modulus (GPa): 358 | Shear modulus (GPa): 341
Young's modulus (GPa): 777 | Highest Young's modulus (GPa): 866
Hardness (GPa): 54 | Energy above hull (eV/atom): 0.12

Primitive Cell

1.000000

7.66831432890008	0.00000000000000	0.00000000000000
-3.83415716445004	6.64095501303169	0.00000000000000
0.00000000000000	0.00000000000000	4.30575952112855

B N

18 18

DIRECT

0.1112440734480273	0.5556220367240137	0.5727712496845659
0.4443779632759866	0.8887559265519728	0.5727712496845659
0.4443779632759865	0.5556220367240136	0.5727712496845659
0.8887559265519727	0.4443779632759863	0.0727712496845661
0.5556220367240134	0.1112440734480272	0.0727712496845661
0.5556220367240134	0.4443779632759864	0.0727712496845661
0.4510542224471950	0.2255271112235974	0.5743059042946190
0.7744728887764025	0.5489457775528052	0.5743059042946190
0.7744728887764024	0.2255271112235974	0.5743059042946190
0.5489457775528050	0.7744728887764025	0.0743059042946190
0.2255271112235974	0.4510542224471948	0.0743059042946190
0.2255271112235975	0.7744728887764025	0.0743059042946190
0.7839030155759448	0.8919515077879725	0.4153949171803329
0.1080484922120276	0.2160969844240551	0.4153949171803329
0.1080484922120275	0.8919515077879724	0.4153949171803329
0.2160969844240552	0.1080484922120275	0.9153949171803328
0.8919515077879724	0.7839030155759449	0.9153949171803328
0.8919515077879725	0.1080484922120276	0.9153949171803328
0.8895374875802635	0.4447687437901318	0.4447865406965026
0.5552312562098681	0.1104625124197364	0.4447865406965026
0.5552312562098680	0.4447687437901318	0.4447865406965026
0.1104625124197365	0.5552312562098682	0.9447865406965025
0.4447687437901319	0.8895374875802636	0.9447865406965025
0.4447687437901320	0.5552312562098682	0.9447865406965025
0.5492311045583040	0.7746155522791520	0.4456581815253364
0.2253844477208479	0.4507688954416958	0.4456581815253364
0.2253844477208481	0.7746155522791521	0.4456581815253364
0.4507688954416960	0.2253844477208480	0.9456581815253363
0.7746155522791521	0.5492311045583042	0.9456581815253363
0.7746155522791519	0.2253844477208479	0.9456581815253363
0.2165387090378070	0.1082693545189035	0.5470831423199006
0.8917306454810965	0.7834612909621931	0.5470831423199006
0.8917306454810965	0.1082693545189035	0.5470831423199006

0.7834612909621930	0.8917306454810965	0.0470831423199008
0.1082693545189035	0.2165387090378069	0.0470831423199008
0.1082693545189035	0.8917306454810965	0.0470831423199008

Stiffness tensor (GPa):

893.899	139.087	85.856	0.020	0.018	0.014
139.087	893.783	85.783	0.018	0.022	-0.006
85.856	85.783	818.309	-0.001	0.018	0.024
0.020	0.018	-0.001	289.387	0.007	0.018
0.018	0.022	0.018	0.007	289.414	0.003
0.014	-0.006	0.024	0.018	0.003	377.928

BN-049

Density (g/cm^3): 3.38 | Space Group: 62
Bulk modulus (GPa): 357 | Shear modulus (GPa): 342
Young's modulus (GPa): 778 | Highest Young's modulus (GPa): 887
Hardness (GPa): 55 | Energy above hull (eV/atom): 0.12

Primitive Cell

1.000000

4.30599388963666	0.00000000000000	0.00000000000000
0.00000000000000	7.68136057587754	0.00000000000000
0.00000000000000	0.00000000000000	4.41978698366001

B N

12 12

DIRECT

0.6706847467745067	0.4116558855617958	0.5880573483456596
0.1706847467745067	0.4116558855617958	0.9119426516543403
0.6706847467745067	0.0883441144382042	0.5880573483456596
0.1706847467745067	0.0883441144382042	0.9119426516543403
0.1725810529299799	0.2500000000000000	0.4161384752305479
0.6725810529299799	0.2500000000000000	0.0838615247694522
0.3293152532254933	0.5883441144382042	0.4119426516543404
0.8293152532254933	0.5883441144382042	0.0880573483456597
0.3293152532254933	0.9116558855617958	0.4119426516543404
0.8293152532254933	0.9116558855617958	0.0880573483456597
0.8274189470700201	0.7500000000000000	0.5838615247694521
0.3274189470700201	0.7500000000000000	0.9161384752305478
0.8011093585724143	0.0882423038564573	0.9117820287232948
0.3011093585724143	0.0882423038564573	0.5882179712767051
0.8011093585724143	0.4117576961435427	0.9117820287232948
0.3011093585724143	0.4117576961435427	0.5882179712767051
0.3005391359728894	0.2500000000000000	0.0858162906479524
0.8005391359728894	0.2500000000000000	0.4141837093520477
0.1988906414275857	0.9117576961435427	0.0882179712767052
0.6988906414275857	0.9117576961435427	0.4117820287232951
0.1988906414275857	0.5882423038564573	0.0882179712767052
0.6988906414275857	0.5882423038564573	0.4117820287232951
0.6994608640271106	0.7500000000000000	0.9141837093520476
0.1994608640271106	0.7500000000000000	0.5858162906479523

Stiffness tensor (GPa):

816.095	90.239	81.845	0.004	-0.007	-0.019
90.239	864.150	140.558	0.009	0.012	-0.017
81.845	140.558	915.841	-0.003	0.002	-0.002
0.004	0.009	-0.003	379.389	0.003	0.000
-0.007	0.012	0.002	0.003	315.720	0.008
-0.019	-0.017	-0.002	0.000	0.008	271.994

BN-050

Density (g/cm^3): 3.38 | Space Group: 36
Bulk modulus (GPa): 358 | Shear modulus (GPa): 340
Young's modulus (GPa): 776 | Highest Young's modulus (GPa): 935
Hardness (GPa): 54 | Energy above hull (eV/atom): 0.11

Primitive Cell

1.000000

1.27413586183549	-6.64698077850814	0.00000000000000
1.27413586183549	6.64698077850814	0.00000000000000
0.00000000000000	0.00000000000000	4.31643652849958

B N

6 6

DIRECT

0.3921253371317047	0.6078746628682954	0.0740098502221622
0.6078746628682954	0.3921253371317047	0.5740098502221622
0.2743446657636437	0.7256553342363563	0.4171680679310524
0.7256553342363563	0.2743446657636437	0.9171680679310523
0.9441693793042019	0.0558306206957981	0.5716514617975532
0.0558306206957981	0.9441693793042019	0.0716514617975532
0.6069525074348529	0.3930474925651471	0.9431758779159269
0.3930474925651471	0.6069525074348529	0.4431758779159269
0.7267006698818068	0.2732993301181932	0.5506091973028391
0.2732993301181932	0.7267006698818068	0.0506091973028391
0.0566325488175967	0.9433674511824033	0.4433855453889433
0.9433674511824033	0.0566325488175967	0.9433855453889433

Stiffness tensor (GPa):

959.791	126.121	81.275	0.006	0.027	0.026
126.121	826.047	113.130	0.001	0.026	0.015
81.275	113.130	807.258	0.007	0.015	0.043
0.006	0.001	0.007	264.021	0.007	-0.004
0.027	0.026	0.015	0.007	334.705	0.003
0.026	0.015	0.043	-0.004	0.003	363.864

BN-051

Density (g/cm^3): 3.38 | Space Group: 34

Bulk modulus (GPa): 329 | Shear modulus (GPa): 298

Young's modulus (GPa): 687 | Highest Young's modulus (GPa): 882

Hardness (GPa): 47 | Energy above hull (eV/atom): 0.42

Primitive Cell

1.000000

4.11847031278805	0.00000000000000	0.00000000000000
0.00000000000000	14.08847705613213	0.00000000000000
0.00000000000000	0.00000000000000	2.51980517101102

B N

12 12

DIRECT

0.1704382596342027	0.4425788733698794	0.7641797853832801
0.6704382596342027	0.0574211266301206	0.2641797853832801
0.3295617403657973	0.9425788733698794	0.2641797853832801
0.8295617403657973	0.5574211266301206	0.7641797853832801
0.0878551574204685	0.2896298489810820	0.4755516331644961
0.5878551574204685	0.2103701510189180	0.9755516331644962
0.4121448425795315	0.7896298489810820	0.9755516331644962
0.9121448425795315	0.7103701510189180	0.4755516331644961
0.3328745584133472	0.6064953205771283	0.2116794519791872
0.8328745584133472	0.8935046794228717	0.7116794519791874
0.1671254415866528	0.1064953205771282	0.7116794519791874
0.6671254415866528	0.3935046794228717	0.2116794519791872
0.2904053101697781	0.0537735274893267	0.2324341198225469
0.7904053101697781	0.4462264725106733	0.7324341198225470
0.2095946898302219	0.5537735274893267	0.7324341198225470
0.7095946898302219	0.9462264725106733	0.2324341198225469
0.3438961527004534	0.2112659634824711	0.5338419812022739
0.8438961527004534	0.2887340365175289	0.0338419812022739
0.1561038472995466	0.7112659634824711	0.0338419812022739
0.6561038472995466	0.7887340365175289	0.5338419812022739
0.2070401726762763	0.8897528310606985	0.7823130222824459
0.7070401726762763	0.6102471689393015	0.2823130222824459
0.2929598273237237	0.3897528310606986	0.2823130222824459
0.7929598273237237	0.1102471689393015	0.7823130222824459

Stiffness tensor (GPa):

841.151	123.028	42.995	0.025	-0.001	-0.023
123.028	717.922	90.112	0.028	0.007	-0.018
42.995	90.112	894.393	0.022	0.029	-0.009
0.025	0.028	0.022	214.524	-0.011	0.026
-0.001	0.007	0.029	-0.011	289.736	0.006
-0.023	-0.018	-0.009	0.026	0.006	288.037

BN-052

Density (g/cm^3): 3.38 | Space Group: 29
Bulk modulus (GPa): 358 | Shear modulus (GPa): 342
Young's modulus (GPa): 778 | Highest Young's modulus (GPa): 888
Hardness (GPa): 55 | Energy above hull (eV/atom): 0.12

Primitive Cell

1.000000

4.42206230109657	0.00000000000000	0.00000000000000
0.00000000000000	7.66948352912601	0.00000000000000
0.00000000000000	0.00000000000000	4.31196344835775

B N

12 12

DIRECT

0.4117642941803770	0.9221284345903478	0.4158033151649729
0.5882357058196230	0.0778715654096522	0.9158033151649730
0.0882357058196230	0.9221284345903478	0.9158033151649730
0.9117642941803770	0.0778715654096522	0.4158033151649729
0.4121159918820849	0.2554131648894395	0.5750612730971124
0.5878840081179151	0.7445868351105605	0.0750612730971123
0.0878840081179151	0.2554131648894395	0.0750612730971123
0.9121159918820849	0.7445868351105605	0.5750612730971124
0.9168601910860925	0.4164082812753064	0.5717230705065180
0.0831398089139075	0.5835917187246936	0.0717230705065179
0.5831398089139075	0.4164082812753064	0.0717230705065179
0.4168601910860925	0.5835917187246936	0.5717230705065180
0.5901811417106146	0.0776719479102570	0.5486784120572218
0.4098188582893854	0.9223280520897430	0.0486784120572217
0.9098188582893854	0.0776719479102570	0.0486784120572217
0.0901811417106146	0.9223280520897430	0.5486784120572218
0.5888924435605518	0.7443868005739334	0.4432780218425610
0.4111075564394482	0.2556131994260666	0.9432780218425612
0.9111075564394482	0.7443868005739334	0.9432780218425612
0.0888924435605518	0.2556131994260666	0.4432780218425610
0.0850506151890671	0.5838226960685359	0.4454559078363031
0.9149493848109329	0.4161773039314641	0.9454559078363032
0.4149493848109329	0.5838226960685359	0.9454559078363032
0.5850506151890671	0.4161773039314641	0.4454559078363031

Stiffness tensor (GPa):

916.078	140.443	82.397	0.003	0.014	0.006
140.443	850.708	104.425	-0.010	0.011	0.002
82.397	104.425	806.781	-0.008	0.003	0.027
0.003	-0.010	-0.008	278.970	0.011	0.004
0.014	0.011	0.003	0.011	319.171	0.000
0.006	0.002	0.027	0.004	0.000	377.311

BN-053

Density (g/cm^3): 3.37 | Space Group: 14
Bulk modulus (GPa): 338 | Shear modulus (GPa): 320
Young's modulus (GPa): 729 | Highest Young's modulus (GPa): 885
Hardness (GPa): 52 | Energy above hull (eV/atom): 0.35

Primitive Cell

1.000000

2.54591011842476	0.00000000000000	0.00000000000000
0.00000000000000	9.39326324486104	0.00000000000000
-1.74594919371694	0.00000000000000	4.09595686467790

B N

8 8

DIRECT

0.4186177837741210	0.8120921704807800	0.4049171739190306
0.4186177837741211	0.6879078295192200	0.9049171739190307
0.1533658585795823	0.5438058935192021	0.3198336074076875
0.1533658585795824	0.9561941064807981	0.8198336074076875
0.5813822162258790	0.1879078295192200	0.5950828260809693
0.5813822162258789	0.3120921704807799	0.0950828260809693
0.8466341414204177	0.4561941064807980	0.6801663925923125
0.8466341414204177	0.0438058935192020	0.1801663925923125
0.1031175582313902	0.6888572480410953	0.1399523063759517
0.1031175582313902	0.8111427519589047	0.6399523063759518
0.3640225167934653	0.9503187012196154	0.2078188782311726
0.3640225167934654	0.5496812987803847	0.7078188782311727
0.8968824417686099	0.3111427519589047	0.8600476936240482
0.8968824417686099	0.1888572480410952	0.3600476936240482
0.6359774832065347	0.0496812987803846	0.7921811217688273
0.6359774832065346	0.4503187012196154	0.2921811217688273

Stiffness tensor (GPa):

882.808	83.145	73.392	0.000	-45.299	0.009
83.145	776.475	177.152	0.028	21.288	0.048
73.392	177.152	728.575	-0.022	-65.791	0.025
0.000	0.028	-0.022	388.180	0.015	-25.308
-45.299	21.288	-65.791	0.015	292.294	0.011
0.009	0.048	0.025	-25.308	0.011	267.450

BN-054

Density (g/cm^3): 3.36 | Space Group: 36

Bulk modulus (GPa): 354 | Shear modulus (GPa): 334

Young's modulus (GPa): 761 | Highest Young's modulus (GPa): 880

Hardness (GPa): 53 | Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

6.39403813661276	-2.21106856679455	0.00000000000000
6.39403813661276	2.21106856679455	0.00000000000000
0.00000000000000	0.00000000000000	4.33563374694633

B N

10 10

DIRECT

0.0413665563378950	0.3654020207994572	0.9178134346617910
0.9586334436621050	0.6345979792005428	0.4178134346617910
0.3654020207994571	0.0413665563378950	0.4178134346617910
0.6345979792005429	0.9586334436621049	0.9178134346617910
0.4346594111233077	0.7592064965605898	0.0768187667374063
0.5653405888766923	0.2407935034394101	0.5768187667374063
0.7592064965605899	0.4346594111233076	0.5768187667374063
0.2407935034394102	0.5653405888766923	0.0768187667374063
0.1667542657392611	0.8332457342607389	0.5733446143352283
0.8332457342607389	0.1667542657392611	0.0733446143352283
0.9561298698293328	0.6371263812216965	0.0510551565737605
0.0438701301706672	0.3628736187783035	0.5510551565737605
0.6371263812216965	0.9561298698293328	0.5510551565737605
0.3628736187783035	0.0438701301706672	0.0510551565737605
0.5640132577351811	0.2420079099391572	0.9446966630446568
0.4359867422648189	0.7579920900608428	0.4446966630446569
0.2420079099391572	0.5640132577351811	0.4446966630446569
0.7579920900608428	0.4359867422648189	0.9446966630446568
0.8363734754386856	0.1636265245613144	0.4458873431030073
0.1636265245613144	0.8363734754386856	0.9458873431030073

Stiffness tensor (GPa):

835.576	141.209	109.961	0.013	0.005	0.016
141.209	910.492	87.525	0.006	0.010	0.010
109.961	87.525	772.508	0.003	-0.001	0.031
0.013	0.006	0.003	315.305	0.013	0.001
0.005	0.010	-0.001	0.013	268.346	-0.006
0.016	0.010	0.031	0.001	-0.006	371.719

BN-055

Density (g/cm^3): 3.36 Space Group: 56

Bulk modulus (GPa): 324 Shear modulus (GPa): 208

Young's modulus (GPa): 515 Highest Young's modulus (GPa): 1148

Hardness (GPa): 24 Energy above hull (eV/atom): 0.93

Primitive Cell

1.000000

2.44038861825417	0.00000000000000	0.00000000000000
0.00000000000000	6.34532081185928	0.00000000000000
0.00000000000000	0.00000000000000	12.67000619853209

B N

16 16

DIRECT

0.2500000000000000	0.2500000000000000	0.2133838332520848
0.7500000000000000	0.7500000000000000	0.7866161667479152
0.7500000000000000	0.7500000000000000	0.2866161667479151
0.2500000000000000	0.2500000000000000	0.7133838332520848
0.9962557712287059	0.9276168268409921	0.1264012260551142
0.0037442287712941	0.0723831731590079	0.8735987739448857
0.5037442287712941	0.5723831731590079	0.1264012260551142
0.4962557712287059	0.4276168268409921	0.8735987739448857
0.0037442287712941	0.4276168268409921	0.3735987739448857
0.9962557712287059	0.5723831731590079	0.6264012260551144
0.4962557712287059	0.0723831731590079	0.3735987739448857
0.5037442287712941	0.9276168268409921	0.6264012260551144
0.2500000000000000	0.7500000000000000	0.4648633965562913
0.7500000000000000	0.2500000000000000	0.5351366034437086
0.7500000000000000	0.2500000000000000	0.0351366034437087
0.2500000000000000	0.7500000000000000	0.9648633965562914
0.2500000000000000	0.7500000000000000	0.2126904523552865
0.7500000000000000	0.2500000000000000	0.7873095476447135
0.7500000000000000	0.2500000000000000	0.2873095476447134
0.2500000000000000	0.7500000000000000	0.7126904523552866
0.0022095038768688	0.4255862509941625	0.1262163227510902
0.9977904961231312	0.5744137490058374	0.8737836772489097
0.4977904961231312	0.0744137490058374	0.1262163227510902
0.5022095038768688	0.9255862509941626	0.8737836772489097
0.9977904961231312	0.9255862509941626	0.3737836772489097
0.0022095038768688	0.0744137490058374	0.6262163227510904
0.5022095038768688	0.5744137490058374	0.3737836772489097
0.4977904961231312	0.4255862509941625	0.6262163227510904
0.2500000000000000	0.2500000000000000	0.4619234354297232
0.7500000000000000	0.7500000000000000	0.5380765645702767
0.7500000000000000	0.7500000000000000	0.0380765645702767
0.2500000000000000	0.2500000000000000	0.9619234354297233

Stiffness tensor (GPa):

1158.379	63.757	61.266	0.075	0.002	0.021
63.757	608.995	186.209	-0.063	0.026	0.028
61.266	186.209	591.323	-0.048	0.011	0.030
0.075	-0.063	-0.048	106.606	-0.001	0.018
0.002	0.026	0.011	-0.001	183.970	0.010
0.021	0.028	0.030	0.018	0.010	189.657

BN-056

Density (g/cm^3): 3.35 Space Group: 173

Bulk modulus (GPa): 353 Shear modulus (GPa): 330

Young's modulus (GPa): 755 Highest Young's modulus (GPa): 841

Hardness (GPa): 52 Energy above hull (eV/atom): 0.14

Primitive Cell

1.000000

6.76095012587270	0.00000000000000	0.00000000000000
-3.38047506293635	5.85515456272536	0.00000000000000
0.00000000000000	0.00000000000000	4.34574044698118

B N

14 14

DIRECT

0.3333333333333333	0.6666666666666666	0.0753119935275031
0.6666666666666667	0.3333333333333333	0.5753119935275030
0.3880374314605245	0.9035158808850410	0.5774000517768769
0.5154784494245165	0.6119625685394755	0.5774000517768769
0.0964841191149590	0.4845215505754835	0.5774000517768769
0.6119625685394755	0.0964841191149590	0.0774000517768769
0.4845215505754835	0.3880374314605245	0.0774000517768769
0.9035158808850410	0.5154784494245165	0.0774000517768769
0.2316858970347362	0.1848367246797058	0.4180302038675417
0.9531508276449696	0.7683141029652638	0.4180302038675417
0.8151632753202942	0.0468491723550304	0.4180302038675417
0.7683141029652638	0.8151632753202942	0.9180302038675416
0.0468491723550304	0.2316858970347362	0.9180302038675416
0.1848367246797058	0.9531508276449696	0.9180302038675416
0.6666666666666666	0.3333333333333333	0.9456317723342604
0.3333333333333333	0.6666666666666666	0.4456317723342605
0.6118070209794944	0.0968795942322804	0.4458798776463996
0.4850725732527861	0.3881929790205056	0.4458798776463996
0.9031204057677196	0.5149274267472139	0.4458798776463996
0.3881929790205056	0.9031204057677196	0.9458798776463995
0.5149274267472139	0.6118070209794944	0.9458798776463995
0.0968795942322804	0.4850725732527861	0.9458798776463995
0.7678403901602513	0.8148483230004677	0.5517086147583122
0.0470079328402164	0.2321596098397487	0.5517086147583122
0.1851516769995323	0.9529920671597836	0.5517086147583122
0.2321596098397487	0.1851516769995323	0.0517086147583124
0.9529920671597836	0.7678403901602513	0.0517086147583124
0.8148483230004677	0.0470079328402164	0.0517086147583124

Stiffness tensor (GPa):

872.323	139.061	100.749	0.011	0.026	0.036
139.061	872.436	100.822	0.019	0.011	0.028
100.749	100.822	763.088	0.000	0.009	0.054
0.011	0.019	0.000	286.166	0.015	0.004

0.026	0.011	0.009	0.015	286.175	0.001
0.036	0.028	0.054	0.004	0.001	367.124

BN-057

Density (g/cm^3): 3.35 | Space Group: 62

Bulk modulus (GPa): 346 | Shear modulus (GPa): 332

Young's modulus (GPa): 755 | Highest Young's modulus (GPa): 861

Hardness (GPa): 54 | Energy above hull (eV/atom): 0.16

Primitive Cell

1.000000

15.57581303074884	0.00000000000000	0.00000000000000
0.00000000000000	2.56235859468887	0.00000000000000
0.00000000000000	0.00000000000000	3.69858683247556

B N

12 12

DIRECT

0.9488768526279994	0.7500000000000000	0.4151546555709007
0.4488768526279994	0.7500000000000000	0.0848453444290993
0.0511231473720006	0.2500000000000000	0.5848453444290993
0.5511231473720006	0.2500000000000000	0.9151546555709007
0.6265004698035251	0.7500000000000000	0.4112513721955509
0.1265004698035250	0.7500000000000000	0.0887486278044491
0.3734995301964749	0.2500000000000000	0.5887486278044491
0.8734995301964749	0.2500000000000000	0.9112513721955509
0.7905547487054158	0.7500000000000000	0.4079944021805337
0.2905547487054156	0.7500000000000000	0.0920055978194663
0.2094452512945842	0.2500000000000000	0.5920055978194663
0.7094452512945842	0.2500000000000000	0.9079944021805337
0.5500578873059158	0.7500000000000000	0.1523034961466763
0.0500578873059156	0.7500000000000000	0.3476965038533237
0.4499421126940842	0.2500000000000000	0.8476965038533237
0.9499421126940842	0.2500000000000000	0.6523034961466763
0.8727876441860960	0.7500000000000000	0.1530388510382235
0.3727876441860960	0.7500000000000000	0.3469611489617765
0.1272123558139040	0.2500000000000000	0.8469611489617765
0.6272123558139040	0.2500000000000000	0.6530388510382235
0.7092031003723545	0.7500000000000000	0.1573415977503665
0.2092031003723545	0.7500000000000000	0.3426584022496335
0.2907968996276455	0.2500000000000000	0.8426584022496335
0.7907968996276455	0.2500000000000000	0.6573415977503665

Stiffness tensor (GPa):

827.522	48.206	192.474	-0.029	0.017	-0.030
48.206	878.921	137.047	-0.015	0.028	-0.046
192.474	137.047	655.227	-0.006	-0.013	-0.054
-0.029	-0.015	-0.006	380.403	-0.001	0.004
0.017	0.028	-0.013	-0.001	353.705	0.000
-0.030	-0.046	-0.054	0.004	0.000	290.616

BN-058

Density (g/cm^3): 3.34 | Space Group: 62

Bulk modulus (GPa): 335 | Shear modulus (GPa): 319

Young's modulus (GPa): 727 | Highest Young's modulus (GPa): 877

Hardness (GPa): 52 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

8.84664075759011	0.00000000000000	0.00000000000000
0.00000000000000	2.57289993268951	0.00000000000000
0.00000000000000	0.00000000000000	4.33808799964959

B N

8 8

DIRECT

0.5466999867214672	0.7500000000000000	0.6700122994546942
0.4533000132785328	0.2500000000000001	0.3299877005453059
0.0466999867214672	0.7500000000000000	0.8299877005453058
0.9533000132785328	0.2500000000000001	0.1700122994546942
0.2072712580933777	0.7500000000000000	0.3359582793472426
0.7927287419066223	0.2500000000000001	0.6640417206527574
0.7072712580933777	0.7500000000000000	0.1640417206527575
0.2927287419066223	0.2500000000000001	0.8359582793472425
0.5464969020274969	0.7500000000000000	0.2929175212403944
0.4535030979725031	0.2500000000000001	0.7070824787596055
0.0464969020274970	0.7500000000000000	0.2070824787596057
0.9535030979725031	0.2500000000000001	0.7929175212403943
0.2094616750142242	0.7500000000000000	0.7064872630794510
0.7905383249857758	0.2500000000000001	0.2935127369205491
0.7094616750142242	0.7500000000000000	0.7935127369205490
0.2905383249857758	0.2500000000000001	0.2064872630794510

Stiffness tensor (GPa):

908.894	137.984	91.182	0.009	-0.003	-0.027
137.984	864.360	66.325	0.011	-0.001	-0.009
91.182	66.325	682.572	0.019	0.010	-0.007
0.009	0.011	0.019	228.019	-0.009	0.018
-0.003	-0.001	0.010	-0.009	303.371	-0.005
-0.027	-0.009	-0.007	0.018	-0.005	375.929

BN-059

Density (g/cm^3): 3.33
Space Group: 136
Bulk modulus (GPa): 354
Shear modulus (GPa): 315
Young's modulus (GPa): 729
Highest Young's modulus (GPa): 945
Hardness (GPa): 47
Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

4.40934852423939	0.00000000000000	0.00000000000000
0.00000000000000	4.40934852423939	0.00000000000000
0.00000000000000	0.00000000000000	2.54454043277733

B N

4 4

DIRECT

0.8258166155077249	0.1741833844922751	0.0000000000000000
0.6741833844922751	0.6741833844922751	0.5000000000000000
0.1741833844922751	0.8258166155077249	0.0000000000000000
0.3258166155077248	0.3258166155077248	0.5000000000000000
0.6874907407194042	0.3125092592805958	0.5000000000000000
0.8125092592805958	0.8125092592805958	0.0000000000000000
0.3125092592805958	0.6874907407194042	0.5000000000000000
0.1874907407194042	0.1874907407194042	0.0000000000000000

Stiffness tensor (GPa):

734.542	170.315	105.688	0.019	0.008	-0.035
170.315	734.591	105.708	-0.017	0.010	-0.028
105.688	105.708	969.713	0.009	0.008	0.002
0.019	-0.017	0.009	333.871	0.008	0.005
0.008	0.010	0.008	0.008	333.881	-0.007
-0.035	-0.028	0.002	0.005	-0.007	244.841

BN-060

Density (g/cm^3): 3.33 | Space Group: 62
Bulk modulus (GPa): 341 | Shear modulus (GPa): 315
Young's modulus (GPa): 723 | Highest Young's modulus (GPa): 864
Hardness (GPa): 50 | Energy above hull (eV/atom): 0.17

Primitive Cell

1.000000

4.35450387081992	0.00000000000000	0.00000000000000
0.00000000000000	5.13963806408939	0.00000000000000
0.00000000000000	0.00000000000000	8.84378274513527

B N

16 16

DIRECT

0.8313146325162912	0.5080277601433912	0.8305800341479705
0.1686853674837088	0.4919722398566088	0.1694199658520294
0.1686853674837088	0.0080277601433911	0.1694199658520294
0.8313146325162912	0.9919722398566089	0.8305800341479705
0.6686853674837088	0.4919722398566088	0.3305800341479705
0.3313146325162912	0.5080277601433912	0.6694199658520295
0.3313146325162912	0.9919722398566089	0.6694199658520295
0.6686853674837088	0.0080277601433911	0.3305800341479705
0.1692019079487621	0.2499999999999999	0.9211195715213853
0.8307980920512379	0.7500000000000000	0.0788804284786146
0.3307980920512379	0.7500000000000000	0.4211195715213853
0.6692019079487621	0.2499999999999999	0.5788804284786147
0.3316324052280981	0.7500000000000000	0.9180322057988268
0.6683675947719019	0.2499999999999999	0.0819677942011732
0.1683675947719019	0.2499999999999999	0.4180322057988268
0.8316324052280981	0.7500000000000000	0.5819677942011732
0.2018141477551048	0.9917590419651385	0.8306277696301905
0.7981858522448952	0.0082409580348615	0.1693722303698095
0.7981858522448952	0.4917590419651384	0.1693722303698095
0.2018141477551048	0.5082409580348616	0.8306277696301905
0.2981858522448952	0.0082409580348615	0.3306277696301904
0.7018141477551048	0.9917590419651385	0.6693722303698095
0.7018141477551048	0.5082409580348616	0.6693722303698095
0.2981858522448952	0.4917590419651384	0.3306277696301904
0.7993592425389597	0.2499999999999999	0.9212112562141019
0.2006407574610403	0.7500000000000000	0.0787887437858980
0.7006407574610403	0.7500000000000000	0.4212112562141019
0.2993592425389597	0.2499999999999999	0.5787887437858981
0.6998927545198010	0.7500000000000000	0.9174790379691711
0.3001072454801990	0.2499999999999999	0.0825209620308289
0.8001072454801990	0.2499999999999999	0.4174790379691710
0.1998927545198010	0.7500000000000000	0.5825209620308289

Stiffness tensor (GPa):

699.338	89.742	93.726	0.000	-0.008	0.022
89.742	838.839	145.309	0.008	-0.000	0.024
93.726	145.309	898.353	-0.010	-0.005	0.035
0.000	0.008	-0.010	368.447	0.002	0.003
-0.008	-0.000	-0.005	0.002	303.121	0.009
0.022	0.024	0.035	0.003	0.009	228.871

BN-061

Density (g/cm^3): 3.33 | Space Group: 14
Bulk modulus (GPa): 327 | Shear modulus (GPa): 289
Young's modulus (GPa): 670 | Highest Young's modulus (GPa): 880
Hardness (GPa): 45 | Energy above hull (eV/atom): 0.30

Primitive Cell

1.000000

2.55293918360935	0.00000000000000	0.00000000000000
0.00000000000000	8.71557926358466	0.00000000000000
-1.18582583189531	0.00000000000000	6.67162535327447

B N

12 12

DIRECT

0.4514808516813680	0.8338699103926014	0.2706966407857786
0.5485191483186320	0.1661300896073986	0.7293033592142214
0.7137356743301584	0.9171478549672825	0.9395833929775085
0.2862643256698417	0.0828521450327175	0.0604166070224915
0.9721906231877132	0.0882176934768849	0.3808995989002453
0.0278093768122867	0.9117823065231151	0.6191004010997547
0.5485191483186320	0.3338699103926013	0.2293033592142214
0.4514808516813679	0.6661300896073986	0.7706966407857786
0.2862643256698416	0.4171478549672825	0.5604166070224915
0.7137356743301584	0.5828521450327175	0.4395833929775086
0.0278093768122868	0.5882176934768849	0.1191004010997547
0.9721906231877132	0.4117823065231151	0.8808995989002453
0.5637174659530431	0.8485520073465517	0.7305467796148876
0.4362825340469569	0.1514479926534483	0.2694532203851124
0.2804115510603974	0.8996976668896987	0.0628842209915347
0.7195884489396025	0.1003023331103013	0.9371157790084653
0.0132880392481443	0.1023133423559484	0.6164054369586162
0.9867119607518557	0.8976866576440516	0.3835945630413838
0.4362825340469569	0.3485520073465516	0.7694532203851124
0.5637174659530431	0.6514479926534483	0.2305467796148877
0.7195884489396026	0.3996976668896988	0.4371157790084653
0.2804115510603974	0.6003023331103013	0.5628842209915347
0.9867119607518557	0.6023133423559484	0.8835945630413838
0.0132880392481443	0.3976866576440516	0.1164054369586163

Stiffness tensor (GPa):

886.346	58.838	115.861	-0.002	25.272	0.013
58.838	629.316	126.357	-0.018	25.788	0.011
115.861	126.357	873.820	0.025	0.781	0.017
-0.002	-0.018	0.025	262.709	0.004	58.629
25.272	25.788	0.781	0.004	348.450	0.002
0.013	0.011	0.017	58.629	0.002	204.387

BN-062

Density (g/cm^3): 3.33 | Space Group: 61
Bulk modulus (GPa): 352 | Shear modulus (GPa): 320
Young's modulus (GPa): 736 | Highest Young's modulus (GPa): 870
Hardness (GPa): 49 | Energy above hull (eV/atom): 0.14

Primitive Cell

1.000000

4.38643936942103	0.00000000000000	0.00000000000000
0.00000000000000	5.09934082431550	0.00000000000000
0.00000000000000	0.00000000000000	4.42608096219867

B N

8 8

DIRECT

0.6709561741451718	0.6335800841157169	0.4128875599399124
0.3290438258548282	0.3664199158842832	0.5871124400600876
0.8290438258548282	0.3664199158842832	0.9128875599399124
0.1709561741451719	0.6335800841157169	0.0871124400600876
0.3290438258548282	0.1335800841157169	0.0871124400600876
0.6709561741451718	0.8664199158842831	0.9128875599399124
0.1709561741451719	0.8664199158842831	0.5871124400600876
0.8290438258548282	0.1335800841157169	0.4128875599399124
0.8065033971495112	0.6344987750815001	0.0920822724524950
0.1934966028504888	0.3655012249185000	0.9079177275475050
0.6934966028504888	0.3655012249185000	0.5920822724524950
0.3065033971495112	0.6344987750815001	0.4079177275475050
0.1934966028504888	0.1344987750815001	0.4079177275475050
0.8065033971495112	0.8655012249184999	0.5920822724524950
0.3065033971495112	0.8655012249184999	0.9079177275475050
0.6934966028504888	0.1344987750815001	0.0920822724524950

Stiffness tensor (GPa):

727.391	142.892	95.866	0.008	0.002	-0.014
142.892	785.603	141.284	0.008	0.000	-0.006
95.866	141.284	902.113	-0.002	0.000	0.002
0.008	0.008	-0.002	360.067	0.006	0.003
0.002	0.000	0.000	0.006	315.453	0.005
-0.014	-0.006	0.002	0.003	0.005	258.311

BN-063

Density (g/cm^3): 3.33 Space Group: 14

Bulk modulus (GPa): 352 Shear modulus (GPa): 318

Young's modulus (GPa): 733 Highest Young's modulus (GPa): 881

Hardness (GPa): 49 Energy above hull (eV/atom): 0.14

Primitive Cell

1.000000

6.75238538402020	0.00000000000000	0.00000000000000
0.00000000000000	4.39224063245115	0.00000000000000
-0.95930666065195	0.00000000000000	5.00642656566798

B N

12 12

DIRECT

0.6081158893528884	0.8285283532012605	0.2685609185357501
0.3918841106471116	0.1714716467987395	0.7314390814642500
0.3918841106471116	0.3285283532012606	0.2314390814642500
0.6081158893528884	0.6714716467987395	0.7685609185357500
0.9418076674861340	0.8288732035158607	0.1195698550352660
0.0581923325138660	0.1711267964841393	0.8804301449647340
0.0581923325138660	0.3288732035158608	0.3804301449647342
0.9418076674861340	0.6711267964841393	0.6195698550352658
0.2753924135329586	0.6710805178643010	0.9360298670460432
0.7246075864670414	0.3289194821356990	0.0639701329539568
0.7246075864670414	0.1710805178643011	0.5639701329539567
0.2753924135329586	0.8289194821356990	0.4360298670460433
0.3951691281285217	0.8075264338910439	0.7355786180226533
0.6048308718714783	0.1924735661089561	0.2644213819773466
0.6048308718714783	0.3075264338910439	0.7644213819773464
0.3951691281285217	0.6924735661089561	0.2355786180226534
0.0614876765640622	0.8067395028172104	0.8813848803328677
0.9385123234359378	0.1932604971827896	0.1186151196671324
0.9385123234359378	0.3067395028172104	0.6186151196671322
0.0614876765640622	0.6932604971827896	0.3813848803328678
0.7278288061261700	0.6921132895831223	0.0674651014170873
0.2721711938738300	0.3078867104168777	0.9325348985829127
0.2721711938738300	0.1921132895831223	0.4325348985829128
0.7278288061261700	0.8078867104168777	0.5674651014170872

Stiffness tensor (GPa):

907.644	100.991	134.203	0.005	-11.286	0.033
100.991	725.676	147.267	-0.011	0.088	0.026
134.203	147.267	778.666	0.009	3.547	0.050
0.005	-0.011	0.009	256.656	0.010	-1.956
-11.286	0.088	3.547	0.010	355.894	0.001
0.033	0.026	0.050	-1.956	0.001	316.661

BN-064

Density (g/cm^3): 3.33 Space Group: 62

Bulk modulus (GPa): 341 Shear modulus (GPa): 316

Young's modulus (GPa): 725 Highest Young's modulus (GPa): 859

Hardness (GPa): 50 Energy above hull (eV/atom): 0.17

Primitive Cell

1.000000

8.83664779199979	0.00000000000000	0.00000000000000
0.00000000000000	5.13752456815925	0.00000000000000
0.00000000000000	0.00000000000000	4.36079481478438

B N

16 16

DIRECT

0.6697862252847785	0.4912957903625241	0.8314727825282643
0.3302137747152215	0.5087042096374759	0.1685272174717357
0.3302137747152215	0.9912957903625241	0.1685272174717357
0.6697862252847785	0.0087042096374759	0.8314727825282643
0.1697862252847786	0.0087042096374759	0.6685272174717358
0.8302137747152215	0.9912957903625241	0.3314727825282641
0.8302137747152215	0.5087042096374759	0.3314727825282641
0.1697862252847786	0.4912957903625241	0.6685272174717358
0.4224161646256137	0.2500000000000000	0.8318323463417358
0.5775838353743863	0.7500000000000000	0.1681676536582642
0.9224161646256137	0.2500000000000000	0.6681676536582644
0.0775838353743863	0.7500000000000000	0.3318323463417356
0.5829765463557511	0.2500000000000000	0.3307722711918636
0.4170234536442489	0.7500000000000000	0.6692277288081363
0.0829765463557512	0.2500000000000000	0.1692277288081363
0.9170234536442489	0.7500000000000000	0.8307722711918637
0.6694631553768438	0.0083137248183089	0.2014760081411922
0.3305368446231562	0.9916862751816911	0.7985239918588077
0.3305368446231562	0.5083137248183089	0.7985239918588077
0.6694631553768438	0.4916862751816911	0.2014760081411922
0.1694631553768438	0.4916862751816911	0.2985239918588077
0.8305368446231562	0.5083137248183089	0.7014760081411924
0.8305368446231562	0.9916862751816911	0.7014760081411924
0.1694631553768438	0.0083137248183089	0.2985239918588077
0.4223230738753511	0.2500000000000000	0.1994569879258914
0.5776769261246489	0.7500000000000000	0.8005430120741086
0.9223230738753511	0.2500000000000000	0.3005430120741086
0.0776769261246489	0.7500000000000000	0.6994569879258914
0.5839529333629258	0.2500000000000000	0.6992416434308666
0.4160470666370742	0.7500000000000000	0.3007583565691334
0.0839529333629256	0.2500000000000000	0.8007583565691334
0.9160470666370742	0.7500000000000000	0.1992416434308666

Stiffness tensor (GPa):

893.703	142.106	101.292	0.004	-0.003	0.012
142.106	837.828	91.898	0.002	0.003	0.032
101.292	91.898	690.339	0.015	0.002	0.037
0.004	0.002	0.015	238.901	-0.002	0.003
-0.003	0.003	0.002	-0.002	301.729	-0.004
0.012	0.032	0.037	0.003	-0.004	368.496

BN-065

Density (g/cm^3): 3.33 | Space Group: 45
Bulk modulus (GPa): 346 | Shear modulus (GPa): 337
Young's modulus (GPa): 764 | Highest Young's modulus (GPa): 994
Hardness (GPa): 55 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

-2.28037329621550	5.16012099959690	2.10663440472290
2.28037329621550	-5.16012099959690	2.10663440472290
2.28037329621550	5.16012099959690	-2.10663440472290

B N

8 8

DIRECT

0.5026212169655960	0.4722599057853443	0.3459524193487220
0.6263074864366223	0.9722599057853443	0.9696386888197481
0.1263074864366223	0.1566687976168741	0.6540475806512780
0.7433494846683102	0.4712874083138392	0.5868873782015533
0.0026212169655961	0.6566687976168740	0.0303613111802517
0.3844000301122858	0.9712874083138392	0.7279379236455290
0.8844000301122859	0.1564621064667568	0.4131126217984466
0.2433494846683102	0.6564621064667568	0.2720620763544710
0.6126238110248159	0.0092183531464979	0.2520880156736656
0.9993042252613800	0.3541194151587098	0.9798560136803760
0.7571303374728324	0.3605357953511503	0.7479119843263344
0.4993042252613800	0.5194482115810040	0.6451848101026700
0.3742634014783338	0.0194482115810039	0.0201439863196240
0.8742634014783337	0.8541194151587098	0.3548151898973300
0.1126238110248159	0.8605357953511503	0.6034054578783179
0.2571303374728323	0.5092183531464980	0.3965945421216820

Stiffness tensor (GPa):

694.861	189.835	42.323	0.021	0.006	0.023
189.835	843.376	65.752	0.017	0.018	0.025
42.323	65.752	1000.348	0.014	0.012	0.032
0.021	0.017	0.014	331.747	0.008	0.010
0.006	0.018	0.012	0.008	281.926	0.002
0.023	0.025	0.032	0.010	0.002	354.537

BN-066

Density (g/cm^3): 3.32	Space Group: 36
Bulk modulus (GPa): 337	Shear modulus (GPa): 314
Young's modulus (GPa): 719	Highest Young's modulus (GPa): 841
Hardness (GPa): 50	Energy above hull (eV/atom): 0.16

Primitive Cell

1.000000

2.56979179350209	-4.40993711885750	0.00000000000000
2.56979179350209	4.40993711885750	0.00000000000000
0.00000000000000	0.00000000000000	4.37586557214800

B N

8 8

DIRECT

0.0706239972103719	0.4102029287294821	0.4259844260233759
0.9293760027896281	0.5897970712705178	0.9259844260233759
0.4102029287294821	0.0706239972103718	0.9259844260233759
0.5897970712705179	0.9293760027896281	0.4259844260233759
0.9162998443699872	0.0837001556300128	0.9295692286872493
0.0837001556300129	0.9162998443699871	0.4295692286872494
0.5767036614899077	0.4232963385100923	0.5928005920707509
0.4232963385100923	0.5767036614899077	0.0928005920707506
0.9283798979427689	0.5895329872589403	0.5575074253491259
0.0716201020572310	0.4104670127410596	0.0575074253491259
0.5895329872589403	0.9283798979427689	0.0575074253491259
0.4104670127410596	0.0716201020572310	0.5575074253491259
0.0831832836704316	0.9168167163295684	0.0564894583365864
0.9168167163295684	0.0831832836704316	0.5564894583365865
0.4216905083708699	0.5783094916291301	0.4541570238968747
0.5783094916291303	0.4216905083708698	0.9541570238968747

Stiffness tensor (GPa):

836.077	141.694	92.846	-0.007	0.017	0.008
141.694	880.581	114.367	-0.006	0.008	0.003
92.846	114.367	652.582	-0.010	-0.000	0.014
-0.007	-0.006	-0.010	302.601	0.007	-0.005
0.017	0.008	-0.000	0.007	249.034	-0.003
0.008	0.003	0.014	-0.005	-0.003	364.721

BN-067

Density (g/cm^3): 3.32 | Space Group: 59

Bulk modulus (GPa): 340 | Shear modulus (GPa): 320

Young's modulus (GPa): 731 | Highest Young's modulus (GPa): 846

Hardness (GPa): 52 | Energy above hull (eV/atom): 0.18

Primitive Cell

1.000000

2.56350064061368	0.00000000000000	0.00000000000000
0.00000000000000	13.01185337454667	0.00000000000000
0.00000000000000	0.00000000000000	3.71907124866990

B N

10 10

DIRECT

0.0000000000000000	0.5987520266530275	0.5892128293465214
0.5000000000000000	0.9012479733469725	0.4107871706534786
0.0000000000000000	0.4012479733469725	0.5892128293465214
0.5000000000000000	0.0987520266530275	0.4107871706534786
0.0000000000000000	0.8111607230427400	0.9151597566548370
0.5000000000000000	0.6888392769572600	0.0848402433451631
0.0000000000000000	0.1888392769572600	0.9151597566548370
0.5000000000000000	0.3111607230427400	0.0848402433451631
0.0000000000000000	0.0000000000000000	0.9087916915443172
0.5000000000000000	0.5000000000000000	0.0912083084556829
0.0000000000000000	0.0979275678553528	0.6526263772199374
0.5000000000000000	0.4020724321446472	0.3473736227800625
0.0000000000000000	0.9020724321446472	0.6526263772199374
0.5000000000000000	0.5979275678553528	0.3473736227800625
0.0000000000000000	0.3098933505816156	0.8482226604341199
0.5000000000000000	0.1901066494183844	0.1517773395658802
0.0000000000000000	0.6901066494183844	0.8482226604341199
0.5000000000000000	0.8098933505816156	0.1517773395658802
0.0000000000000000	0.5000000000000000	0.8425894855391214
0.5000000000000000	0.0000000000000000	0.1574105144608786

Stiffness tensor (GPa):

868.379	51.172	131.527	-0.007	-0.023	-0.059
51.172	808.144	195.403	-0.009	-0.024	-0.064
131.527	195.403	631.496	-0.014	-0.023	-0.073
-0.007	-0.009	-0.014	330.326	0.025	-0.003
-0.023	-0.024	-0.023	0.025	366.730	0.002
-0.059	-0.064	-0.073	-0.003	0.002	286.460

BN-068

Density (g/cm^3): 3.32 | Space Group: 2

Bulk modulus (GPa): 337 | Shear modulus (GPa): 315

Young's modulus (GPa): 720 | Highest Young's modulus (GPa): 826

Hardness (GPa): 50 | Energy above hull (eV/atom): 0.40

Primitive Cell

1.000000

4.23235457897146	0.00000000000000	0.00000000000000
-1.41550578332086	4.04881420222526	0.00000000000000
-1.33181764231612	-1.87753464202937	10.15579175173950

B N

14 14

DIRECT

0.3592750772296786	0.8007280196354103	0.9226670179693096
0.6407249227703213	0.1992719803645897	0.0773329820306904
0.8675704342546565	0.6945236201855919	0.2915310772367943
0.1324295657453435	0.3054763798144081	0.7084689227632057
0.6912085262000084	0.4426185874954284	0.8607038642248579
0.3087914737999916	0.5573814125045716	0.1392961357751421
0.5492101367881478	0.3163943481774683	0.5619183487813443
0.4507898632118522	0.6836056518225317	0.4380816512186557
0.9345894357034192	0.8778660766042868	0.0770733335395284
0.0654105642965808	0.1221339233957132	0.9229266664604716
0.4341092210457572	0.1075282379740871	0.2903813698144186
0.5658907789542429	0.8924717620259129	0.7096186301855814
0.0050998687386030	0.7367703683731438	0.5616227637301107
0.9949001312613970	0.2632296316268562	0.4383772362698893
0.3628811080574063	0.2839552761592056	0.4174834325580883
0.6371188919425936	0.7160447238407944	0.5825165674419117
0.8698617314377987	0.1878482154901076	0.7970309600665864
0.1301382685622013	0.8121517845098924	0.2029690399334136
0.6947417127414727	0.9459888201321194	0.3544260134802667
0.3052582872585273	0.0540111798678806	0.6455739865197333
0.5456708969081044	0.7987292567868836	0.0627836605678665
0.4543291030918956	0.2012707432131164	0.9372163394321336
0.9412743794722187	0.3628916555359954	0.5828993554213532
0.0587256205277813	0.6371083444640047	0.4171006445786468
0.4321186013084320	0.6155849271381201	0.7938708656210720
0.5678813986915680	0.3844150728618799	0.2061291343789280
0.0103224440821844	0.2566588530491166	0.0622563927789147
0.9896775559178156	0.7433411469508835	0.9377436072210853

Stiffness tensor (GPa):

788.993	109.300	148.324	1.308	15.464	23.346
109.300	709.703	154.233	31.483	5.887	40.486
148.324	154.233	716.967	2.339	2.760	-25.308
1.308	31.483	2.339	338.492	7.989	10.940

15.464	5.887	2.760	7.989	317.727	10.619
23.346	40.486	-25.308	10.940	10.619	325.531

BN-069

Density (g/cm^3): 3.31 | Space Group: 2
Bulk modulus (GPa): 346 | Shear modulus (GPa): 218
Young's modulus (GPa): 540 | Highest Young's modulus (GPa): 766
Hardness (GPa): 24 | Energy above hull (eV/atom): 0.52

Primitive Cell

1.000000

2.54119937634875	0.00000000000000	0.00000000000000
-0.00008297382713	6.12625739591133	0.00000000000000
-0.00002263778262	-0.00000107416674	11.18916638315945

B N

14 14

DIRECT

0.5000001391641504	0.8285153618061842	0.1115442636033192
0.4999998604897729	0.6714840906180453	0.3884563706443027
0.9999996085405448	0.4999999012286824	0.2066589057821962
0.4999992303369649	0.1714845347703836	0.1115440953256827
0.5000007696194466	0.3285160124071090	0.3884565407073955
0.0000003913332659	0.0000000975827164	0.2933419442286728
-0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000001395102271	0.3285159093819547	0.6115436293556973
0.4999998608358495	0.1714846381938158	0.8884557363966809
0.9999996086667341	0.9999999024172836	0.7066580557713271
0.4999992303805534	0.6714839875928910	0.6115434592926046
0.5000007696630351	0.8285154652296164	0.8884559046743172
0.0000003914594552	0.5000000987713176	0.7933410942178039
-0.0000000000000000	0.0000000000000000	0.5000000000000000
0.9999934778453873	0.6871072011238286	0.1111499239323290
0.0000065208902806	0.8128934779032999	0.3888506352509685
0.4999995135411385	0.5000001456555293	0.2849946832013416
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.0000047012689929	0.3128926046193131	0.1111499375118017
0.9999953003086448	0.1871067138133259	0.3888506232526744
0.5000004861791210	0.9999998528558973	0.2150064251691085
0.9999934791097194	0.1871065220967001	0.6111493647490315
0.0000065221546127	0.3128927988761714	0.8888500760676710
0.4999995138208790	0.0000001471441027	0.7849935748308915
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.0000046996913552	0.8128932861866741	0.6111493767473256
0.9999952987310071	0.6871073953806869	0.8888500624881983
0.5000004864588614	0.4999998543444707	0.7150053167986584

Stiffness tensor (GPa):

748.045	139.622	149.983	-0.008	-0.269	0.034
139.622	798.963	101.680	-0.021	-0.201	0.068
149.983	101.680	782.445	-0.084	0.370	0.038
-0.008	-0.021	-0.084	193.049	0.002	0.086

-0.269	-0.201	0.370	0.002	241.949	-0.138
0.034	0.068	0.038	0.086	-0.138	103.454

BN-070

Density (g/cm^3): 3.30 | Space Group: 14
Bulk modulus (GPa): 328 | Shear modulus (GPa): 299
Young's modulus (GPa): 688 | Highest Young's modulus (GPa): 876
Hardness (GPa): 47 | Energy above hull (eV/atom): 0.39

Primitive Cell

1.000000

2.52783293873078	0.00000000000000	0.00000000000000
0.00000000000000	4.02443962248577	0.00000000000000
-2.47094865049433	0.00000000000000	14.75241404975683

B N

12 12

DIRECT

0.1979659303889756	0.0861591269052154	0.9460892356196702
0.8020340696110244	0.9138408730947846	0.0539107643803298
0.8020340696110244	0.5861591269052154	0.5539107643803298
0.1979659303889755	0.4138408730947846	0.4460892356196702
0.2026994748991378	0.1818979183013106	0.7760186809027594
0.7973005251008622	0.8181020816986894	0.2239813190972406
0.7973005251008622	0.6818979183013106	0.7239813190972406
0.2026994748991377	0.3181020816986894	0.2760186809027594
0.5965288734173584	0.5953085562292504	0.8736526709611905
0.4034711265826416	0.4046914437707496	0.1263473290388095
0.4034711265826417	0.0953085562292504	0.6263473290388095
0.5965288734173584	0.9046914437707496	0.3736526709611905
0.6986172794950045	0.8630809531698822	0.9458268330890365
0.3013827205049955	0.1369190468301178	0.0541731669109635
0.3013827205049955	0.3630809531698822	0.5541731669109635
0.6986172794950045	0.6369190468301178	0.4458268330890365
0.3508817379096656	0.7982585372252899	0.7787874754982493
0.6491182620903344	0.2017414627747101	0.2212125245017507
0.6491182620903344	0.2982585372252899	0.7212125245017507
0.3508817379096655	0.7017414627747101	0.2787874754982493
0.1361849447138859	0.3589933394702119	0.8742919897058425
0.8638150552861141	0.6410066605297882	0.1257080102941575
0.8638150552861141	0.8589933394702118	0.6257080102941575
0.1361849447138858	0.1410066605297881	0.3742919897058425

Stiffness tensor (GPa):

884.521	60.756	63.246	-0.007	-1.049	-0.022
60.756	710.318	196.527	-0.017	-39.508	-0.018
63.246	196.527	720.299	-0.007	34.275	0.001
-0.007	-0.017	-0.007	318.630	0.019	-35.315
-1.049	-39.508	34.275	0.019	244.696	-0.004
-0.022	-0.018	0.001	-35.315	-0.004	302.498

BN-071

Density (g/cm^3): 3.29 | Space Group: 19

Bulk modulus (GPa): 329 | Shear modulus (GPa): 275

Young's modulus (GPa): 644 | Highest Young's modulus (GPa): 710

Hardness (GPa): 40 | Energy above hull (eV/atom): 0.55

Primitive Cell

1.000000

4.28266251101053	0.00000000000000	0.00000000000000
0.00000000000000	4.94052783754287	0.00000000000000
0.00000000000000	0.00000000000000	7.10296737809832

B N

12 12

DIRECT

0.5804649103427708	0.4934233811159063	0.6918951638837731
0.9195350896572292	0.5065766188840937	0.1918951638837731
0.4195350896572292	0.9934233811159063	0.8081048361162269
0.0804649103427708	0.0065766188840937	0.3081048361162268
0.0526329060734492	0.2343374403962211	0.6316208224262843
0.4473670939265508	0.7656625596037789	0.1316208224262842
0.9473670939265508	0.7343374403962211	0.8683791775737157
0.5526329060734492	0.2656625596037789	0.3683791775737157
0.3387851019809636	0.3718968675675491	0.0423634112579807
0.1612148980190364	0.6281031324324509	0.5423634112579807
0.6612148980190364	0.8718968675675491	0.4576365887420192
0.8387851019809636	0.1281031324324509	0.9576365887420193
0.5651579693578430	0.4752911128586002	0.1979252634791430
0.9348420306421570	0.5247088871413998	0.6979252634791431
0.4348420306421570	0.9752911128586002	0.3020747365208569
0.0651579693578430	0.0247088871413998	0.8020747365208569
0.0435220338864764	0.2099209330775265	0.1320125910780703
0.4564779661135236	0.7900790669224735	0.6320125910780703
0.9564779661135236	0.7099209330775265	0.3679874089219297
0.5435220338864764	0.2900790669224735	0.8679874089219297
0.3617162964186653	0.3603115498463734	0.5374168313873009
0.1382837035813347	0.6396884501536266	0.0374168313873009
0.6382837035813347	0.8603115498463734	0.9625831686126991
0.8617162964186653	0.1396884501536266	0.4625831686126990

Stiffness tensor (GPa):

742.003	107.649	169.351	0.004	0.035	-0.014
107.649	594.067	212.378	0.014	-0.014	-0.011
169.351	212.378	653.514	0.035	-0.008	-0.011
0.004	0.014	0.035	282.980	0.087	0.011
0.035	-0.014	-0.008	0.087	308.923	0.014
-0.014	-0.011	-0.011	0.011	0.014	297.349

BN-072

Density (g/cm^3): 3.29 | Space Group: 38

Bulk modulus (GPa): 344 | Shear modulus (GPa): 305

Young's modulus (GPa): 707 | Highest Young's modulus (GPa): 976

Hardness (GPa): 46 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

2.60301386872854	0.00000000000000	0.00000000000000
0.00000000000000	5.70682480534935	2.11097111269157
0.00000000000000	-5.70682480534935	2.11097111269157

B N

5 5

DIRECT

0.5000000000000000	0.3709757281487588	0.9995430732841892
0.5000000000000000	0.9995430732841892	0.3709757281487588
0.0000000000000000	0.1585600214912254	0.1585600214912254
0.0000000000000000	0.5697461184793051	0.8086793245844686
0.0000000000000000	0.8086793245844686	0.5697461184793051
0.5000000000000000	0.6259971196707693	0.0014666672590310
0.5000000000000000	0.0014666672590309	0.6259971196707693
0.0000000000000000	0.8321149305912665	0.8321149305912665
0.0000000000000000	0.4348165126012595	0.1981005039283465
0.0000000000000000	0.1981005039283465	0.4348165126012595

Stiffness tensor (GPa):

988.102	102.879	36.431	0.016	-0.015	0.018
102.879	965.994	88.689	0.013	-0.018	0.047
36.431	88.689	724.404	-0.016	-0.006	-0.009
0.016	0.013	-0.016	202.636	0.013	0.017
-0.015	-0.018	-0.006	0.013	215.730	0.004
0.018	0.047	-0.009	0.017	0.004	370.195

BN-073

Density (g/cm^3): 3.28 | Space Group: 14
Bulk modulus (GPa): 318 | Shear modulus (GPa): 281
Young's modulus (GPa): 651 | Highest Young's modulus (GPa): 778
Hardness (GPa): 44 | Energy above hull (eV/atom): 0.42

Primitive Cell

1.000000

2.53478409321847	0.00000000000000	0.00000000000000
0.00000000000000	14.73215394008576	0.00000000000000
-2.14627373363790	0.00000000000000	4.03665122258030

B N

12 12

DIRECT

0.1608121266516120	0.9463665762381824	0.4130446851854968
0.8391878733483880	0.0536334237618176	0.5869553148145032
0.8391878733483880	0.4463665762381823	0.0869553148145031
0.1608121266516120	0.5536334237618176	0.9130446851854969
0.8604809983635788	0.7780189586690883	0.3214442025905560
0.1395190016364212	0.2219810413309117	0.6785557974094441
0.1395190016364211	0.2780189586690884	0.1785557974094439
0.8604809983635788	0.7219810413309117	0.8214442025905561
0.1862468027364073	0.8745196468185997	0.9050547742377023
0.8137531972635927	0.1254803531814003	0.0949452257622977
0.8137531972635927	0.3745196468185998	0.5949452257622978
0.1862468027364072	0.6254803531814003	0.4050547742377021
0.8627640862668060	0.9455820843548535	0.6364810609513076
0.1372359137331940	0.0544179156451465	0.3635189390486923
0.1372359137331940	0.4455820843548535	0.8635189390486924
0.8627640862668060	0.5544179156451465	0.1364810609513076
0.1891447986952831	0.7809027483746944	0.7016021758471678
0.8108552013047169	0.2190972516253056	0.2983978241528323
0.8108552013047169	0.2809027483746944	0.7983978241528323
0.1891447986952831	0.7190972516253056	0.2016021758471677
0.8618587530075315	0.8755793629907673	0.1387031378029963
0.1381412469924686	0.1244206370092327	0.8612968621970036
0.1381412469924685	0.3755793629907673	0.3612968621970036
0.8618587530075315	0.6244206370092327	0.6387031378029964

Stiffness tensor (GPa):

777.568	27.109	101.591	0.009	-26.057	-0.037
27.109	679.458	208.319	-0.018	40.313	-0.002
101.591	208.319	743.708	0.031	5.398	0.025
0.009	-0.018	0.031	311.149	-0.022	0.591
-26.057	40.313	5.398	-0.022	294.133	-0.030
-0.037	-0.002	0.025	0.591	-0.030	209.838

BN-074

Density (g/cm^3): 3.28 | Space Group: 62

Bulk modulus (GPa): 329 | Shear modulus (GPa): 307

Young's modulus (GPa): 703 | Highest Young's modulus (GPa): 829

Hardness (GPa): 50 | Energy above hull (eV/atom): 0.21

Primitive Cell

1.000000

10.43712025524715	0.00000000000000	0.00000000000000
0.00000000000000	2.56476594847341	0.00000000000000
0.00000000000000	0.00000000000000	3.75924345625960

B N

8 8

DIRECT

0.5762514631505504	0.2500000000000000	0.9142042917389395
0.9237485368494496	0.7500000000000000	0.4142042917389395
0.6871955613572263	0.7500000000000000	0.4106213698250543
0.8128044386427739	0.2500000000000000	0.9106213698250543
0.4237485368494495	0.7500000000000000	0.0857957082610605
0.0762514631505504	0.2500000000000000	0.5857957082610605
0.3128044386427738	0.2500000000000000	0.5893786301749457
0.1871955613572260	0.7500000000000000	0.0893786301749457
0.9250295690936516	0.2500000000000000	0.6493859216187602
0.5749704309063484	0.7500000000000000	0.1493859216187601
0.8115720702789089	0.7500000000000000	0.1509452793550414
0.6884279297210911	0.2500000000000000	0.6509452793550414
0.0749704309063483	0.7500000000000000	0.3506140783812398
0.4250295690936516	0.2500000000000000	0.8506140783812398
0.1884279297210911	0.2500000000000000	0.8490547206449586
0.3115720702789088	0.7500000000000000	0.3490547206449586

Stiffness tensor (GPa):

778.951	55.193	200.598	-0.039	0.017	-0.022
55.193	854.028	122.095	-0.013	-0.010	-0.033
200.598	122.095	584.680	-0.020	0.005	-0.036
-0.039	-0.013	-0.020	348.697	-0.037	-0.000
0.017	-0.010	0.005	-0.037	325.736	0.002
-0.022	-0.033	-0.036	-0.000	0.002	277.778

BN-075

Density (g/cm^3): 3.27 | Space Group: 39
Bulk modulus (GPa): 338 | Shear modulus (GPa): 308
Young's modulus (GPa): 709 | Highest Young's modulus (GPa): 981
Hardness (GPa): 48 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

4.62376674371767	0.00000000000000	0.00000000000000
0.00000000000000	3.87682426436357	2.10663555825183
0.00000000000000	-3.87682426436357	2.10663555825183

B N

6 6

DIRECT

0.1559540275334354	0.7204491742750565	0.9079741240000185
0.8440459724665645	0.2204491742750563	0.4079741240000184
0.8440459724665645	0.9079741240000183	0.7204491742750563
0.1559540275334354	0.4079741240000184	0.2204491742750564
0.3469891353042498	0.0649342132449244	0.5649342132449244
0.6530108646957502	0.5649342132449244	0.0649342132449244
0.8234026707578423	0.2803544898513359	0.0904537775350902
0.1765973292421577	0.7803544898513359	0.5904537775350902
0.1765973292421577	0.0904537775350902	0.2803544898513359
0.8234026707578423	0.5904537775350902	0.7803544898513359
0.6659674615157305	0.9358342282002732	0.4358342282002732
0.3340325384842695	0.4358342282002732	0.9358342282002732

Stiffness tensor (GPa):

640.290	200.849	40.981	0.020	0.032	-0.003
200.849	821.784	67.996	0.005	-0.000	0.026
40.981	67.996	987.238	0.011	0.009	0.040
0.020	0.005	0.011	331.991	0.006	0.013
0.032	-0.000	0.009	0.006	259.935	-0.013
-0.003	0.026	0.040	0.013	-0.013	272.109

BN-076

Density (g/cm^3): 3.27 | Space Group: 14

Bulk modulus (GPa): 331 | Shear modulus (GPa): 293

Young's modulus (GPa): 679 | Highest Young's modulus (GPa): 835

Hardness (GPa): 45 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

6.79636268967285	0.00000000000000	0.00000000000000
0.00000000000000	4.45192525614421	0.00000000000000
-0.98122789172166	0.00000000000000	5.00030148092431

B N

12 12

DIRECT

0.3841586486398189	0.8346942879311670	0.4640986283203290
0.6158413513601810	0.1653057120688330	0.5359013716796710
0.6158413513601810	0.3346942879311670	0.0359013716796710
0.3841586486398189	0.6653057120688330	0.9640986283203290
0.0581828101429048	0.6699913105251319	0.6486242039964748
0.9418171898570952	0.3300086894748681	0.3513757960035252
0.9418171898570952	0.1699913105251318	0.8513757960035252
0.0581828101429048	0.8300086894748681	0.1486242039964747
0.7263153411357569	0.8315531653075668	0.2956961352722143
0.2736846588642431	0.1684468346924332	0.7043038647277857
0.2736846588642431	0.3315531653075667	0.2043038647277857
0.7263153411357569	0.6684468346924332	0.7956961352722143
0.6140149825236533	0.8024144527971292	0.5360676067730396
0.3859850174763467	0.1975855472028708	0.4639323932269604
0.3859850174763467	0.3024144527971293	0.9639323932269604
0.6140149825236533	0.6975855472028708	0.0360676067730394
0.9399562656703665	0.6941074617357477	0.3504469331888473
0.0600437343296335	0.3058925382642523	0.6495530668111527
0.0600437343296335	0.1941074617357477	0.1495530668111527
0.9399562656703665	0.8058925382642523	0.8504469331888473
0.2718936294319746	0.8055640976457324	0.7041570162345347
0.7281063705680254	0.1944359023542676	0.2958429837654653
0.7281063705680254	0.3055640976457323	0.7958429837654653
0.2718936294319746	0.6944359023542676	0.2041570162345347

Stiffness tensor (GPa):

859.418	92.516	143.925	-0.002	10.724	0.002
92.516	593.880	147.153	-0.018	-3.341	-0.012
143.925	147.153	798.286	-0.001	14.559	0.010
-0.002	-0.018	-0.001	258.495	0.009	18.894
10.724	-3.341	14.559	0.009	349.954	0.001
0.002	-0.012	0.010	18.894	0.001	254.919

BN-077

Density (g/cm^3): 3.27 | Space Group: 63

Bulk modulus (GPa): 339 | Shear modulus (GPa): 307

Young's modulus (GPa): 707 | Highest Young's modulus (GPa): 845

Hardness (GPa): 48 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

1.28334880343700	-4.27979887729632	0.00000000000000
1.28334880343700	4.27979887729632	0.00000000000000
0.00000000000000	0.00000000000000	6.88470692837816

B N

6 6

DIRECT

0.5452796437731380	0.4547203562268620	0.7500000000000000
0.8374830701771712	0.1625169298228288	0.5595816081062133
0.1625169298228288	0.8374830701771712	0.4404183918937868
0.4547203562268620	0.5452796437731380	0.2500000000000000
0.8374830701771712	0.1625169298228288	0.9404183918937868
0.1625169298228288	0.8374830701771712	0.0595816081062130
0.9362020567410473	0.0637979432589527	0.7500000000000000
0.3500935395926900	0.6499064604073100	0.4331037086426300
0.6499064604073100	0.3500935395926900	0.5668962913573699
0.0637979432589526	0.9362020567410474	0.2500000000000000
0.3500935395926900	0.6499064604073100	0.0668962913573699
0.6499064604073100	0.3500935395926900	0.9331037086426301

Stiffness tensor (GPa):

851.756	79.119	92.484	-0.014	-0.001	0.001
79.119	640.135	222.500	-0.007	0.004	-0.001
92.484	222.500	779.498	0.006	-0.000	0.009
-0.014	-0.007	0.006	386.912	0.036	0.012
-0.001	0.004	-0.000	0.036	269.204	-0.007
0.001	-0.001	0.009	0.012	-0.007	282.774

BN-078

Density (g/cm^3): 3.27 | Space Group: 19

Bulk modulus (GPa): 330 | Shear modulus (GPa): 295

Young's modulus (GPa): 682 | Highest Young's modulus (GPa): 828

Hardness (GPa): 46 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

4.43340523925494	0.00000000000000	0.00000000000000
0.00000000000000	4.45365742118019	0.00000000000000
0.00000000000000	0.00000000000000	7.66756698267233

B N

12 12

DIRECT

0.8299014346275615	0.1649989084533461	0.5785218440684226
0.3299014346275615	0.3350010915466539	0.4214781559315774
0.1700985653724385	0.6649989084533461	0.9214781559315774
0.6700985653724385	0.8350010915466539	0.0785218440684226
0.8407305059205687	0.1689010232975159	0.2558015718290585
0.3407305059205687	0.3310989767024841	0.7441984281709415
0.1592694940794313	0.6689010232975159	0.2441984281709415
0.6592694940794313	0.8310989767024841	0.7558015718290585
0.6801771444651190	0.6674989734253018	0.4182264112918039
0.1801771444651190	0.8325010265746982	0.5817735887081961
0.3198228555348810	0.1674989734253018	0.0817735887081961
0.8198228555348810	0.3325010265746981	0.9182264112918039
0.1715323491632863	0.3049060868573616	0.9209019295544714
0.6715323491632863	0.1950939131426383	0.0790980704455286
0.8284676508367137	0.8049060868573616	0.5790980704455286
0.3284676508367137	0.6950939131426384	0.4209019295544714
0.1624256191658238	0.3016917858618497	0.2433450373524184
0.6624256191658238	0.1983082141381502	0.7566549626475816
0.8375743808341762	0.8016917858618497	0.2566549626475816
0.3375743808341762	0.6983082141381503	0.7433450373524184
0.3176952077431265	0.8044733055876081	0.0831591536185086
0.8176952077431265	0.6955266944123919	0.9168408463814914
0.6823047922568735	0.3044733055876080	0.4168408463814914
0.1823047922568735	0.1955266944123919	0.5831591536185086

Stiffness tensor (GPa):

808.237	127.084	137.217	-0.012	0.003	0.018
127.084	583.618	112.816	0.004	0.029	0.016
137.217	112.816	866.004	0.016	0.010	0.034
-0.012	0.004	0.016	274.893	0.002	0.001
0.003	0.029	0.010	0.002	345.937	0.001
0.018	0.016	0.034	0.001	0.001	246.113

BN-079

Density (g/cm^3): 3.27 | Space Group: 14
Bulk modulus (GPa): 332 | Shear modulus (GPa): 291
Young's modulus (GPa): 675 | Highest Young's modulus (GPa): 879
Hardness (GPa): 44 | Energy above hull (eV/atom): 0.18

Primitive Cell

1.000000

6.76417355899317	0.00000000000000	0.00000000000000
0.00000000000000	4.47143717830367	0.00000000000000
-0.93017804650798	0.00000000000000	5.00544869361342

B N

12 12

DIRECT

0.2273890790289505	0.3302566363307463	0.8171565219789696
0.7726109209710494	0.6697433636692537	0.1828434780210304
0.7726109209710494	0.8302566363307463	0.6828434780210304
0.2273890790289505	0.1697433636692537	0.3171565219789696
0.5588315035991562	0.1708905146122035	0.1470941118884799
0.4411684964008437	0.8291094853877965	0.8529058881115201
0.4411684964008437	0.6708905146122035	0.3529058881115201
0.5588315035991562	0.3291094853877965	0.6470941118884799
0.8841699575513390	0.3348852030622785	0.4759478605248963
0.1158300424486610	0.6651147969377216	0.5240521394751037
0.1158300424486610	0.8348852030622784	0.0240521394751037
0.8841699575513390	0.1651147969377215	0.9759478605248963
0.7715665445716484	0.3078267009302318	0.1780877197252997
0.2284334554283516	0.6921732990697682	0.8219122802747003
0.2284334554283516	0.8078267009302318	0.3219122802747003
0.7715665445716484	0.1921732990697682	0.6780877197252997
0.4399988611254874	0.1911035303512272	0.8475493676556014
0.5600011388745125	0.8088964696487728	0.1524506323443986
0.5600011388745125	0.6911035303512272	0.6524506323443986
0.4399988611254874	0.3088964696487728	0.3475493676556014
0.1148405279191900	0.3049983662113180	0.5190345589433483
0.8851594720808100	0.6950016337886820	0.4809654410566517
0.8851594720808100	0.8049983662113180	0.9809654410566517
0.1148405279191900	0.1950016337886820	0.0190345589433483

Stiffness tensor (GPa):

883.333	109.872	133.360	-0.006	-37.326	0.004
109.872	581.881	156.045	-0.003	1.189	-0.006
133.360	156.045	768.045	0.000	-12.635	0.013
-0.006	-0.003	0.000	246.496	0.016	-36.570
-37.326	1.189	-12.635	0.016	343.756	-0.000
0.004	-0.006	0.013	-36.570	-0.000	279.264

BN-080

Density (g/cm^3): 3.26 | Space Group: 14
Bulk modulus (GPa): 330 | Shear modulus (GPa): 292
Young's modulus (GPa): 676 | Highest Young's modulus (GPa): 824
Hardness (GPa): 45 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

7.68873570538975	0.00000000000000	0.00000000000000
0.00000000000000	4.41188776321922	0.00000000000000
-0.00426912781408	0.00000000000000	4.46632008441319

B N

12 12

DIRECT

0.0846995529139735	0.9052700120348136	0.6614393094464384
0.9153004470860264	0.0947299879651864	0.3385606905535617
0.9153004470860264	0.4052700120348137	0.8385606905535616
0.0846995529139735	0.5947299879651863	0.1614393094464384
0.2573529648385458	0.4125867862356242	0.8266079439514198
0.7426470351614542	0.5874132137643758	0.1733920560485802
0.7426470351614542	0.9125867862356241	0.6733920560485802
0.2573529648385458	0.0874132137643760	0.3266079439514198
0.4115558121201527	0.9129573218555981	0.8283382237393542
0.5884441878798473	0.0870426781444019	0.1716617762606459
0.5884441878798473	0.4129573218555983	0.6716617762606458
0.4115558121201527	0.5870426781444018	0.3283382237393542
0.0838941561689842	0.5958562599630893	0.8034750382836089
0.9161058438310158	0.4041437400369107	0.1965249617163912
0.9161058438310158	0.0958562599630895	0.6965249617163911
0.0838941561689842	0.9041437400369106	0.3034750382836089
0.2578609145696015	0.0923319368482514	0.6919718130878558
0.7421390854303984	0.9076680631517486	0.3080281869121442
0.7421390854303984	0.5923319368482513	0.8080281869121442
0.2578609145696015	0.4076680631517487	0.1919718130878559
0.4111123655596057	0.5922417573069599	0.6915367424043515
0.5888876344403943	0.4077582426930401	0.3084632575956486
0.5888876344403943	0.0922417573069601	0.8084632575956485
0.4111123655596057	0.9077582426930400	0.1915367424043515

Stiffness tensor (GPa):

781.386	140.613	130.901	0.003	2.998	0.010
140.613	869.198	127.752	0.011	-0.973	-0.004
130.901	127.752	569.080	-0.016	-0.800	0.011
0.003	0.011	-0.016	300.887	0.011	0.322
2.998	-0.973	-0.800	0.011	227.900	-0.001
0.010	-0.004	0.011	0.322	-0.001	347.891

BN-081

Density (g/cm^3): 3.26 | Space Group: 36

Bulk modulus (GPa): 329 | Shear modulus (GPa): 293

Young's modulus (GPa): 677 | Highest Young's modulus (GPa): 825

Hardness (GPa): 45 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

3.84590327340693	-2.20565161883361	0.00000000000000
3.84590327340693	2.20565161883361	0.00000000000000
0.00000000000000	0.00000000000000	4.46817906116747

B N

6 6

DIRECT

0.1557299488720485	0.8442700511279515	0.9095603008434812
0.8442700511279515	0.1557299488720485	0.4095603008434812
0.8356787929208791	0.5104563229435140	0.0765126279897853
0.1643212070791208	0.4895436770564860	0.5765126279897853
0.5104563229435140	0.8356787929208791	0.5765126279897853
0.4895436770564860	0.1643212070791208	0.0765126279897853
0.8461053327646741	0.1538946672353259	0.0536131920285358
0.1538946672353259	0.8461053327646741	0.5536131920285358
0.1696469227343030	0.4846599743070184	0.9419006243428401
0.8303530772656970	0.5153400256929817	0.4419006243428401
0.4846599743070185	0.1696469227343030	0.4419006243428401
0.5153400256929817	0.8303530772656971	0.9419006243428401

Stiffness tensor (GPa):

782.859	139.737	132.394	0.003	-0.005	-0.005
139.737	868.933	126.043	0.077	-0.003	-0.022
132.394	126.043	562.344	0.007	-0.004	0.009
0.003	0.077	0.007	298.505	0.012	-0.005
-0.005	-0.003	-0.004	0.012	233.651	-0.000
-0.005	-0.022	0.009	-0.005	-0.000	348.539

BN-082

Density (g/cm^3): 3.26 | Space Group: 56

Bulk modulus (GPa): 335 | Shear modulus (GPa): 304

Young's modulus (GPa): 700 | Highest Young's modulus (GPa): 835

Hardness (GPa): 48 | Energy above hull (eV/atom): 0.24

Primitive Cell

1.000000

4.58968333155225	0.00000000000000	0.00000000000000
0.00000000000000	10.30688929834825	0.00000000000000
0.00000000000000	0.00000000000000	4.28240776404996

B N

16 16

DIRECT

0.5976079633951983	0.4340566343109162	0.6679611707138893
0.4023920366048017	0.5659433656890838	0.3320388292861108
0.0976079633951983	0.5659433656890838	0.8320388292861108
0.9023920366048017	0.4340566343109162	0.1679611707138892
0.5942721013634589	0.6790519128936712	0.8281324465855195
0.4057278986365411	0.3209480871063288	0.1718675534144804
0.0942721013634589	0.3209480871063288	0.6718675534144805
0.9057278986365411	0.6790519128936712	0.3281324465855195
0.9023920366048017	0.0659433656890838	0.6679611707138893
0.0976079633951983	0.9340566343109162	0.3320388292861108
0.4023920366048017	0.9340566343109162	0.8320388292861108
0.5976079633951983	0.0659433656890838	0.1679611707138892
0.9057278986365411	0.8209480871063288	0.8281324465855195
0.0942721013634589	0.1790519128936712	0.1718675534144804
0.4057278986365411	0.1790519128936712	0.6718675534144805
0.5942721013634589	0.8209480871063288	0.3281324465855195
0.4114798436005578	0.5671386296899132	0.6978402335887741
0.5885201563994422	0.4328613703100868	0.3021597664112258
0.9114798436005578	0.4328613703100868	0.8021597664112259
0.0885201563994422	0.5671386296899132	0.1978402335887741
0.4221198557789148	0.3231893631220928	0.8023181954042204
0.5778801442210852	0.6768106368779072	0.1976818045957795
0.9221198557789148	0.6768106368779072	0.6976818045957796
0.0778801442210852	0.3231893631220928	0.3023181954042204
0.0885201563994422	0.9328613703100868	0.6978402335887741
0.9114798436005578	0.0671386296899132	0.3021597664112258
0.5885201563994422	0.0671386296899132	0.8021597664112259
0.4114798436005578	0.9328613703100868	0.1978402335887741
0.0778801442210852	0.1768106368779072	0.8023181954042204
0.9221198557789148	0.8231893631220928	0.1976818045957795
0.5778801442210852	0.8231893631220928	0.6976818045957796
0.4221198557789148	0.1768106368779072	0.3023181954042204

Stiffness tensor (GPa):

684.636	201.252	62.453	0.022	-0.000	0.017
201.252	760.613	97.426	-0.005	0.014	0.028
62.453	97.426	849.703	0.007	0.007	0.030
0.022	-0.005	0.007	278.239	0.004	0.005
-0.000	0.014	0.007	0.004	279.141	-0.000
0.017	0.028	0.030	0.005	-0.000	335.236

BN-083

Density (g/cm^3): 3.25 | Space Group: 11

Bulk modulus (GPa): 313 | Shear modulus (GPa): 258

Young's modulus (GPa): 607 | Highest Young's modulus (GPa): 811

Hardness (GPa): 38 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.43729844497983	0.00000000000000	0.00000000000000
0.00000000000000	5.13779848681716	0.00000000000000
-0.00470922692313	0.00000000000000	4.44756117530683

B N

8 8

DIRECT

0.3315820481975788	0.7500000000000000	0.6537878252981808
0.6684179518024211	0.2500000000000000	0.3462121747018192
0.6700257715240190	0.0072264888935807	0.8280401661977566
0.3299742284759810	0.9927735111064193	0.1719598338022434
0.3299742284759810	0.5072264888935807	0.1719598338022434
0.6700257715240190	0.4927735111064193	0.8280401661977566
0.1641560585055837	0.2500000000000000	0.6693121958371826
0.8358439414944163	0.7500000000000000	0.3306878041628174
0.7050273459880740	0.7500000000000000	0.6543476175232248
0.2949726540119260	0.2500000000000000	0.3456523824767752
0.2953808902973517	0.4921171136133097	0.8285808370959349
0.7046191097026483	0.5078828863866903	0.1714191629040651
0.7046191097026483	0.9921171136133097	0.1714191629040651
0.2953808902973517	0.0078828863866903	0.8285808370959349
0.8001444458448970	0.2500000000000000	0.6679132921075039
0.1998555541551030	0.7500000000000000	0.3320867078924961

Stiffness tensor (GPa):

539.170	96.019	96.627	-0.003	-0.736	-0.039
96.019	842.898	135.782	0.010	5.694	-0.009
96.627	135.782	845.091	-0.001	-3.874	-0.010
-0.003	0.010	-0.001	354.967	0.002	5.669
-0.736	5.694	-3.874	0.002	172.665	0.011
-0.039	-0.009	-0.010	5.669	0.011	192.832

BN-084

Density (g/cm^3): 3.25 | Space Group: 164
Bulk modulus (GPa): 311 | Shear modulus (GPa): 252
Young's modulus (GPa): 595 | Highest Young's modulus (GPa): 805
Hardness (GPa): 37 | Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

5.14000155475720	0.00000000000000	0.00000000000000
-2.57000077737860	4.45137192191125	0.00000000000000
0.00000000000000	0.00000000000000	4.43418836402827

B N

8 8

DIRECT

0.3333333333333333	0.6666666666666666	0.3345963678869395
0.6666666666666667	0.3333333333333334	0.6654036321130605
0.8278761805700460	0.6557523611400919	0.1697634043221864
0.1721238194299540	0.3442476388599081	0.8302365956778136
0.3442476388599081	0.1721238194299540	0.1697634043221864
0.6557523611400919	0.8278761805700460	0.8302365956778136
0.8278761805700460	0.1721238194299540	0.1697634043221864
0.1721238194299540	0.8278761805700460	0.8302365956778136
0.6666666666666666	0.3333333333333333	0.2995897646113106
0.3333333333333334	0.6666666666666667	0.7004102353886894
0.1719262531696968	0.3438525063393937	0.2052477474174799
0.8280737468303032	0.6561474936606063	0.7947522525825200
0.6561474936606063	0.8280737468303032	0.2052477474174799
0.3438525063393937	0.1719262531696968	0.7947522525825200
0.1719262531696968	0.8280737468303032	0.2052477474174799
0.8280737468303032	0.1719262531696968	0.7947522525825200

Stiffness tensor (GPa):

839.066	135.388	98.122	6.004	0.014	0.033
135.388	839.224	98.143	-6.107	0.005	0.029
98.122	98.143	531.431	-0.018	0.030	0.052
6.004	-6.107	-0.018	174.484	0.008	-0.004
0.014	0.005	0.030	0.008	174.417	6.044
0.033	0.029	0.052	-0.004	6.044	351.544

BN-085

Density (g/cm^3): 3.25 Space Group: 60

Bulk modulus (GPa): 327 Shear modulus (GPa): 305

Young's modulus (GPa): 699 Highest Young's modulus (GPa): 813

Hardness (GPa): 49 Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

10.41601866223842	0.00000000000000	0.00000000000000
0.00000000000000	4.55649999388801	0.00000000000000
0.00000000000000	0.00000000000000	4.28015302581594

B N

16 16

DIRECT

0.0753567187561530	0.1510942893533069	0.5807053129629945
0.4246432812438470	0.3489057106466931	0.0807053129629947
0.0753567187561530	0.8489057106466931	0.0807053129629947
0.4246432812438470	0.6510942893533069	0.5807053129629945
0.3117463199158143	0.8414558501387147	0.0778625280940509
0.1882536800841857	0.6585441498612853	0.5778625280940508
0.3117463199158143	0.1585441498612853	0.5778625280940508
0.1882536800841857	0.3414558501387148	0.0778625280940509
0.9246432812438470	0.8489057106466931	0.4192946870370055
0.5753567187561530	0.6510942893533069	0.9192946870370053
0.9246432812438470	0.1510942893533069	0.9192946870370053
0.5753567187561530	0.3489057106466931	0.4192946870370055
0.6882536800841857	0.1585441498612853	0.9221374719059491
0.8117463199158143	0.3414558501387148	0.4221374719059492
0.6882536800841857	0.8414558501387147	0.4221374719059492
0.8117463199158143	0.6585441498612853	0.9221374719059491
0.4228969743348244	0.3331575590835615	0.4463976522054651
0.0771030256651756	0.1668424409164385	0.9463976522054650
0.4228969743348244	0.6668424409164385	0.9463976522054650
0.0771030256651756	0.8331575590835615	0.4463976522054651
0.1870433591015772	0.6648705647321952	0.9487637557125329
0.3129566408984228	0.8351294352678048	0.4487637557125331
0.1870433591015772	0.3351294352678048	0.4487637557125331
0.3129566408984228	0.1648705647321953	0.9487637557125329
0.5771030256651756	0.6668424409164385	0.5536023477945349
0.9228969743348244	0.8331575590835615	0.0536023477945350
0.5771030256651756	0.3331575590835615	0.0536023477945350
0.9228969743348244	0.1668424409164385	0.5536023477945349
0.8129566408984228	0.3351294352678048	0.0512362442874671
0.6870433591015772	0.1648705647321953	0.5512362442874670
0.8129566408984228	0.6648705647321952	0.5512362442874670
0.6870433591015772	0.8351294352678048	0.0512362442874671

Stiffness tensor (GPa):

775.550	186.521	98.395	0.012	-0.000	0.024
186.521	690.406	46.133	0.008	-0.000	0.023
98.395	46.133	826.603	-0.021	-0.020	0.050
0.012	0.008	-0.021	281.438	0.005	0.013
-0.000	-0.000	-0.020	0.005	289.128	0.002
0.024	0.023	0.050	0.013	0.002	314.424

BN-086

Density (g/cm^3): 3.24 | Space Group: 62
Bulk modulus (GPa): 307 | Shear modulus (GPa): 278
Young's modulus (GPa): 641 | Highest Young's modulus (GPa): 810
Hardness (GPa): 45 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.45584830567793	0.00000000000000	0.00000000000000
0.00000000000000	5.13853623506885	0.00000000000000
0.00000000000000	0.00000000000000	8.88413942551134

B N

16 16

DIRECT

0.8358823578910730	0.7500000000000000	0.8258595673733824
0.3358823578910730	0.7500000000000000	0.6741404326266176
0.1641176421089270	0.2500000000000000	0.1741404326266176
0.6641176421089270	0.2500000000000000	0.3258595673733824
0.6688901639593523	0.0092322960075941	0.5860469381793449
0.1688901639593523	0.0092322960075941	0.9139530618206551
0.1688901639593523	0.4907677039924058	0.9139530618206551
0.6688901639593523	0.4907677039924058	0.5860469381793449
0.3311098360406476	0.9907677039924059	0.4139530618206551
0.8311098360406477	0.9907677039924059	0.0860469381793449
0.8311098360406477	0.5092322960075941	0.0860469381793449
0.3311098360406476	0.5092322960075941	0.4139530618206551
0.3337684837062844	0.7500000000000000	0.1644439489375222
0.8337684837062844	0.7500000000000000	0.3355560510624778
0.6662315162937156	0.2500000000000000	0.8355560510624778
0.1662315162937155	0.2500000000000000	0.6644439489375222
0.7029177417353960	0.7500000000000000	0.6712361620285034
0.2029177417353960	0.7500000000000000	0.8287638379714966
0.2970822582646039	0.2500000000000000	0.3287638379714966
0.7970822582646040	0.2500000000000000	0.1712361620285034
0.7971514415631629	0.4916339584315325	0.9138997403775859
0.2971514415631628	0.4916339584315325	0.5861002596224141
0.2971514415631628	0.0083660415684674	0.5861002596224141
0.7971514415631629	0.0083660415684674	0.9138997403775859
0.2028485584368371	0.5083660415684674	0.0861002596224141
0.7028485584368371	0.5083660415684674	0.4138997403775859
0.7028485584368371	0.9916339584315326	0.4138997403775859
0.2028485584368371	0.9916339584315326	0.0861002596224141
0.2016142301094987	0.7500000000000000	0.3328609551535968
0.7016142301094987	0.7500000000000000	0.1671390448464032
0.7983857698905013	0.2500000000000000	0.6671390448464032
0.2983857698905012	0.2500000000000000	0.8328609551535968

Stiffness tensor (GPa):

503.961	95.140	102.719	0.006	0.011	0.014
95.140	844.336	136.253	0.012	0.006	0.019
102.719	136.253	837.861	-0.005	0.004	0.026
0.006	0.012	-0.005	350.366	0.007	0.003
0.011	0.006	0.004	0.007	232.127	0.003
0.014	0.019	0.026	0.003	0.003	225.465

BN-087

Density (g/cm^3): 3.24
Space Group: 55
Bulk modulus (GPa): 306
Shear modulus (GPa): 274
Young's modulus (GPa): 633
Highest Young's modulus (GPa): 804
Hardness (GPa): 44
Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.45209558146876	0.00000000000000	0.00000000000000
0.00000000000000	8.89145922839378	0.00000000000000
0.00000000000000	0.00000000000000	5.14143383654668

B N

16 16

DIRECT

0.6662089209621238	0.1736283163002529	0.0000000000000000
0.3337910790378762	0.8263716836997471	0.0000000000000000
0.8337910790378762	0.6736283163002529	0.0000000000000000
0.1662089209621238	0.3263716836997471	0.0000000000000000
0.3317978807252222	0.0861631663457608	0.2598596229375438
0.6682021192747778	0.9138368336542392	0.7401403770624562
0.6682021192747778	0.9138368336542392	0.2598596229375438
0.3317978807252222	0.0861631663457608	0.7401403770624562
0.1682021192747778	0.5861631663457608	0.7401403770624562
0.8317978807252222	0.4138368336542392	0.2598596229375438
0.8317978807252222	0.4138368336542392	0.7401403770624562
0.1682021192747778	0.5861631663457608	0.2598596229375438
0.1672072827702090	0.8346550208794720	0.5000000000000001
0.8327927172297910	0.1653449791205280	0.5000000000000001
0.3327927172297910	0.3346550208794721	0.5000000000000001
0.6672072827702090	0.6653449791205280	0.5000000000000001
0.2978991144314573	0.1709964243156324	0.0000000000000000
0.7021008855685427	0.8290035756843676	0.0000000000000000
0.2021008855685427	0.6709964243156324	0.0000000000000000
0.7978991144314573	0.3290035756843676	0.0000000000000000
0.7039774194856537	0.0862840240542930	0.7415424516948199
0.2960225805143463	0.9137159759457070	0.2584575483051800
0.2960225805143463	0.9137159759457070	0.7415424516948199
0.7039774194856537	0.0862840240542930	0.2584575483051800
0.7960225805143463	0.5862840240542930	0.2584575483051800
0.2039774194856538	0.4137159759457070	0.7415424516948199
0.2039774194856538	0.4137159759457070	0.2584575483051800
0.7960225805143463	0.5862840240542930	0.7415424516948199
0.7972605426828004	0.8326710934838113	0.5000000000000001
0.2027394573171996	0.1673289065161887	0.5000000000000001
0.7027394573171996	0.3326710934838113	0.5000000000000001
0.2972605426828006	0.6673289065161887	0.5000000000000001

Stiffness tensor (GPa):

496.476	103.264	98.173	0.023	-0.002	0.025
103.264	834.632	135.542	0.005	0.002	0.022
98.173	135.542	839.696	0.014	-0.001	0.041
0.023	0.005	0.014	348.261	0.008	0.005
-0.002	0.002	-0.001	0.008	216.156	-0.000
0.025	0.022	0.041	0.005	-0.000	231.429

BN-088

Density (g/cm^3): 3.23 | Space Group: 14
Bulk modulus (GPa): 320 | Shear modulus (GPa): 278
Young's modulus (GPa): 647 | Highest Young's modulus (GPa): 845
Hardness (GPa): 43 | Energy above hull (eV/atom): 0.21

Primitive Cell

1.000000

4.44398611430899	0.00000000000000	0.00000000000000
0.00000000000000	4.51559114343015	0.00000000000000
-0.04288109146286	0.00000000000000	5.08645283025691

B N

8 8

DIRECT

0.6597854922307977	0.8316039633580794	0.2602456753678801
0.3402145077692023	0.1683960366419206	0.7397543246321199
0.3402145077692023	0.3316039633580793	0.2397543246321198
0.6597854922307977	0.6683960366419206	0.7602456753678801
0.1725990982150272	0.6646749563201486	0.5056857688683023
0.8274009017849728	0.3353250436798513	0.4943142311316976
0.8274009017849728	0.1646749563201486	0.9943142311316977
0.1725990982150272	0.8353250436798514	0.0056857688683023
0.3402972669504474	0.8068059497464963	0.7363457491914587
0.6597027330495526	0.1931940502535036	0.2636542508085413
0.6597027330495526	0.3068059497464963	0.7636542508085413
0.3402972669504474	0.6931940502535037	0.2363457491914586
0.8272039188199589	0.6937429752204425	0.4902831934109605
0.1727960811800411	0.3062570247795575	0.5097168065890394
0.1727960811800411	0.1937429752204425	0.0097168065890394
0.8272039188199589	0.8062570247795575	0.9902831934109606

Stiffness tensor (GPa):

835.278	109.017	142.134	-0.005	33.864	-0.010
109.017	511.727	156.558	-0.027	-0.462	-0.010
142.134	156.558	783.445	0.014	19.548	0.012
-0.005	-0.027	0.014	258.381	-0.002	39.943
33.864	-0.462	19.548	-0.002	346.984	0.000
-0.010	-0.010	0.012	39.943	0.000	246.768

BN-089

Density (g/cm^3): 3.22	Space Group: 17
Bulk modulus (GPa): 252	Shear modulus (GPa): 193
Young's modulus (GPa): 461	Highest Young's modulus (GPa): 752
Hardness (GPa): 29	Energy above hull (eV/atom): 1.16

Primitive Cell

1.000000

2.98264661029500	0.00000000000000	0.00000000000000
0.00000000000000	2.98303471696673	0.00000000000000
0.00000000000000	0.00000000000000	5.75244989851170

B N

4 4

DIRECT

0.5000000000000000	0.1479011041266840	0.7500000000000000
0.1478826064334737	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.8520988958733160	0.2499999999999999
0.8521173935665263	0.5000000000000000	0.5000000000000001
0.0000000000000000	0.4118914392710930	0.7500000000000000
0.4118591991267371	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5881085607289069	0.2499999999999999
0.5881408008732629	0.0000000000000000	0.5000000000000001

Stiffness tensor (GPa):

309.015	117.112	284.779	0.007	0.042	-0.044
117.112	308.758	284.851	-0.067	-0.017	-0.045
284.779	284.851	743.039	-0.058	0.093	-0.036
0.007	-0.067	-0.058	377.429	-0.012	-0.005
0.042	-0.017	0.093	-0.012	377.360	0.001
-0.044	-0.045	-0.036	-0.005	0.001	190.110

BN-090

Density (g/cm^3): 3.22 | Space Group: 88
Bulk modulus (GPa): 286 | Shear modulus (GPa): 252
Young's modulus (GPa): 585 | Highest Young's modulus (GPa): 659
Hardness (GPa): 41 | Energy above hull (eV/atom): 0.59

Primitive Cell

1.000000

-3.94383541681208	3.94383541681208	3.29076412098456
3.94383541681208	-3.94383541681208	3.29076412098456
3.94383541681208	3.94383541681208	-3.29076412098456

B N

16 16

DIRECT

0.4855755361143701	0.2522253473422947	0.4478027596258408
0.2644244638856299	0.9977746526577052	0.0521972403741591
0.8044225877164539	0.0377727764885292	0.5521972403741591
0.9455774122835461	0.2122272235114708	0.9478027596258409
0.7877727764885293	0.7355755361143701	0.7333501887720754
0.9622272235114708	0.5144244638856299	0.7666498112279247
0.0022253473422948	0.0544225877164539	0.2666498112279246
0.7477746526577053	0.1955774122835461	0.2333501887720754
0.3840453876471922	0.7155312434230392	0.1420087682888956
0.3659546123528077	0.5344687565769608	0.3579912317111043
0.5735224751341436	0.2420366193582966	0.8579912317111044
0.1764775248658565	0.0079633806417034	0.6420087682888957
0.4655312434230392	0.8235224751341435	0.8314858557758469
0.2844687565769608	0.4264775248658564	0.6685141442241530
0.9920366193582966	0.6340453876471923	0.1685141442241531
0.7579633806417034	0.6159546123528078	0.3314858557758470
0.9734787722624687	0.0159816056976829	0.7464410549355252
0.7765212277375313	0.2340183943023172	0.7535589450644750
0.2695405507621578	0.2270377173269437	0.2535589450644750
0.4804594492378422	0.0229622826730564	0.2464410549355251
0.7659816056976829	0.5195405507621578	0.5425028334352142
0.9840183943023171	0.7304594492378422	0.9574971665647858
0.9770377173269436	0.2234787722624687	0.4574971665647858
0.7729622826730564	0.0265212277375313	0.0425028334352142
0.1514883781185237	0.5198508788591510	0.1737456054160894
0.5985116218814763	0.7301491211408488	0.3262543945839105
0.3461052734430616	0.9777427727024341	0.8262543945839105
0.4038947265569384	0.2722572272975658	0.6737456054160895
0.7277427727024343	0.4014883781185237	0.1316374992593726
0.0222572272975658	0.8485116218814763	0.3683625007406274
0.2698508788591510	0.5961052734430616	0.8683625007406274
0.4801491211408490	0.6538947265569384	0.6316374992593726

Stiffness tensor (GPa):

653.018	157.755	71.893	0.018	0.011	-3.321
157.755	653.096	71.927	-0.017	0.006	3.353
71.893	71.927	671.406	-0.007	-0.004	0.033
0.018	-0.017	-0.007	246.510	-0.005	-0.000
0.011	0.006	-0.004	-0.005	246.494	0.007
-3.321	3.353	0.033	-0.000	0.007	217.442

BN-091

Density (g/cm^3): 3.21 | Space Group: 59
Bulk modulus (GPa): 316 | Shear modulus (GPa): 280
Young's modulus (GPa): 649 | Highest Young's modulus (GPa): 803
Hardness (GPa): 44 | Energy above hull (eV/atom): 0.27

Primitive Cell

1.000000

2.56841637673377	0.00000000000000	0.00000000000000
0.00000000000000	7.86725324694911	0.00000000000000
0.00000000000000	0.00000000000000	3.81411161876266

B N

6 6

DIRECT

0.5000000000000000	0.4999999999999999	0.9129757639786390
0.0000000000000000	0.0000000000000000	0.0870242360213610
0.0000000000000000	0.3504738030695786	0.4151747630953083
0.5000000000000000	0.1495261969304214	0.5848252369046917
0.0000000000000000	0.6495261969304214	0.4151747630953083
0.5000000000000000	0.8504738030695786	0.5848252369046917
0.5000000000000000	0.0000000000000000	0.8528285698086437
0.0000000000000000	0.4999999999999999	0.1471714301913563
0.0000000000000000	0.8489918207228304	0.3504346109584174
0.5000000000000000	0.6510081792771696	0.6495653890415827
0.0000000000000000	0.1510081792771696	0.3504346109584174
0.5000000000000000	0.3489918207228305	0.6495653890415827

Stiffness tensor (GPa):

826.043	57.321	111.891	-0.025	-0.020	-0.095
57.321	748.952	198.113	-0.010	0.010	-0.101
111.891	198.113	552.069	-0.008	0.011	-0.094
-0.025	-0.010	-0.008	252.632	0.017	-0.000
-0.020	0.010	0.011	0.017	320.220	-0.002
-0.095	-0.101	-0.094	-0.000	-0.002	269.927

BN-092

Density (g/cm^3): 3.20 | Space Group: 12
Bulk modulus (GPa): 313 | Shear modulus (GPa): 259
Young's modulus (GPa): 608 | Highest Young's modulus (GPa): 829
Hardness (GPa): 38 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

2.21723163289635	-3.83078504736467	0.00000000000000
2.21723163289635	3.83078504736467	0.00000000000000
-0.05527523917075	0.00000000000000	4.54709119100770

B N

6 6

DIRECT

0.3324582081959205	0.0119504521780490	0.6671840425968807
0.6675417918040796	0.9880495478219511	0.3328159574031194
0.9880495478219511	0.6675417918040796	0.3328159574031194
0.0119504521780490	0.3324582081959205	0.6671840425968807
0.3219261809754163	0.3219261809754161	0.1635962982040018
0.6780738190245839	0.6780738190245839	0.8364037017959982
0.6632857666333871	0.9842891493556754	0.6972864113257888
0.3367142333666129	0.0157108506443246	0.3027135886742112
0.0157108506443246	0.3367142333666129	0.3027135886742112
0.9842891493556754	0.6632857666333871	0.6972864113257888
0.6791410735131982	0.6791410735131982	0.1907789349134763
0.3208589264868018	0.3208589264868017	0.8092210650865237

Stiffness tensor (GPa):

767.686	126.523	138.551	-0.007	-14.813	0.005
126.523	870.970	121.259	-0.017	-2.662	0.002
138.551	121.259	484.925	-0.020	-2.361	0.009
-0.007	-0.017	-0.020	220.671	0.013	-1.949
-14.813	-2.662	-2.361	0.013	204.042	0.006
0.005	0.002	0.009	-1.949	0.006	329.621

BN-093

Density (g/cm^3): 3.20 | Space Group: 14

Bulk modulus (GPa): 310 | Shear modulus (GPa): 267

Young's modulus (GPa): 622 | Highest Young's modulus (GPa): 782

Hardness (GPa): 41 | Energy above hull (eV/atom): 0.24

Primitive Cell

1.000000

4.55214973053445	0.00000000000000	0.00000000000000
0.00000000000000	4.42654792381304	0.00000000000000
-4.46358556128318	0.00000000000000	7.68077711447964

B N

12 12

DIRECT

0.4924260098796190	0.8361401227499322	0.6592283217925263
0.5075739901203810	0.1638598772500678	0.3407716782074736
0.5075739901203811	0.3361401227499323	0.8407716782074737
0.4924260098796190	0.6638598772500679	0.1592283217925263
0.0055008875207325	0.3479863365053254	0.1682994230472565
0.9944991124792675	0.6520136634946745	0.8317005769527435
0.9944991124792675	0.8479863365053255	0.3317005769527435
0.0055008875207326	0.1520136634946745	0.6682994230472565
0.1611846167954897	0.3260573687309876	0.4951704868756609
0.8388153832045103	0.6739426312690124	0.5048295131243391
0.8388153832045102	0.8260573687309876	0.0048295131243390
0.1611846167954898	0.1739426312690124	0.9951704868756610
0.1457759222041135	0.1602834767697298	0.3398586551623787
0.8542240777958865	0.8397165232302702	0.6601413448376212
0.8542240777958865	0.6602834767697299	0.1601413448376212
0.1457759222041135	0.3397165232302702	0.8398586551623788
0.6383451085656675	0.6507566381312007	0.8312672015046356
0.3616548914343325	0.3492433618687993	0.1687327984953644
0.3616548914343326	0.1507566381312006	0.6687327984953644
0.6383451085656674	0.8492433618687993	0.3312672015046356
0.2043602883855120	0.6700133922638363	0.5052073256328355
0.7956397116144880	0.3299866077361637	0.4947926743671645
0.7956397116144880	0.1700133922638362	0.9947926743671646
0.2043602883855120	0.8299866077361637	0.0052073256328353

Stiffness tensor (GPa):

468.003	123.377	133.855	0.006	6.061	0.010
123.377	829.563	141.253	-0.007	-5.892	0.010
133.855	141.253	781.667	0.008	-15.301	0.037
0.006	-0.007	0.008	341.520	0.004	-5.443
6.061	-5.892	-15.301	0.004	225.939	0.010
0.010	0.010	0.037	-5.443	0.010	239.696

BN-094

Density (g/cm^3): 3.19 | Space Group: 18
Bulk modulus (GPa): 310 | Shear modulus (GPa): 266
Young's modulus (GPa): 620 | Highest Young's modulus (GPa): 804
Hardness (GPa): 41 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

4.43714040330530	0.00000000000000	0.00000000000000
0.00000000000000	4.56537722530714	0.00000000000000
0.00000000000000	0.00000000000000	7.64734692340064

B N

12 12

DIRECT

0.8227680266879811	0.8321058925222078	0.5841159423810511
0.1772319733120189	0.1678941074777922	0.5841159423810511
0.6772319733120189	0.3321058925222077	0.4158840576189489
0.3227680266879811	0.6678941074777922	0.4158840576189489
0.6713640689611138	0.1619892734745480	0.0755696646109130
0.3286359310388862	0.8380107265254519	0.0755696646109130
0.8286359310388862	0.6619892734745481	0.9244303353890870
0.1713640689611138	0.3380107265254519	0.9244303353890870
0.8284489321431769	0.8328977923632601	0.2575642635493223
0.1715510678568231	0.1671022076367399	0.2575642635493223
0.6715510678568231	0.3328977923632601	0.7424357364506777
0.3284489321431769	0.6671022076367399	0.7424357364506777
0.6818122578124051	0.6896409935935321	0.4168653212742996
0.3181877421875949	0.3103590064064678	0.4168653212742996
0.8181877421875949	0.1896409935935321	0.5831346787257004
0.1818122578124051	0.8103590064064679	0.5831346787257004
0.8247763996962566	0.3038794750740918	0.9228758477482080
0.1752236003037434	0.6961205249259081	0.9228758477482080
0.6752236003037434	0.8038794750740919	0.0771241522517920
0.3247763996962565	0.1961205249259081	0.0771241522517920
0.6775552690506326	0.6939655895933541	0.7434861267867134
0.3224447309493674	0.3060344104066459	0.7434861267867134
0.8224447309493674	0.1939655895933541	0.2565138732132866
0.1775552690506326	0.8060344104066459	0.2565138732132866

Stiffness tensor (GPa):

762.018	135.885	130.601	-0.006	-0.002	0.009
135.885	460.149	136.010	-0.011	0.011	0.020
130.601	136.010	855.245	0.009	-0.005	0.029
-0.006	-0.011	0.009	269.819	0.001	-0.002
-0.002	0.011	-0.005	0.001	326.390	0.005
0.009	0.020	0.029	-0.002	0.005	211.185

BN-095

Density (g/cm^3): 3.19 | Space Group: 14

Bulk modulus (GPa): 308 | Shear modulus (GPa): 261

Young's modulus (GPa): 611 | Highest Young's modulus (GPa): 787

Hardness (GPa): 40 | Energy above hull (eV/atom): 0.22

Primitive Cell

1.000000

6.80593412928984	0.00000000000000	0.00000000000000
0.00000000000000	4.58881816830335	0.00000000000000
-1.01471222661534	0.00000000000000	4.97146323494951

B N

12 12

DIRECT

0.1063103256178577	0.6701429210149585	0.2873056667357601
0.8936896743821423	0.3298570789850415	0.7126943332642399
0.8936896743821423	0.1701429210149585	0.2126943332642399
0.1063103256178577	0.8298570789850415	0.7873056667357601
0.4478631213687501	0.6613201593352067	0.1209505477056760
0.5521368786312499	0.3386798406647933	0.8790494522943240
0.5521368786312499	0.1613201593352067	0.3790494522943240
0.4478631213687501	0.8386798406647933	0.6209505477056760
0.7825644281318365	0.6642926091397537	0.9493506267395251
0.2174355718681635	0.3357073908602463	0.0506493732604749
0.2174355718681635	0.1642926091397539	0.5506493732604749
0.7825644281318365	0.8357073908602463	0.4493506267395251
0.8937213212262056	0.6910258877713772	0.7073809872386684
0.1062786787737944	0.3089741122286228	0.2926190127613316
0.1062786787737944	0.1910258877713771	0.7926190127613316
0.8937213212262056	0.8089741122286228	0.2073809872386683
0.5514488958565533	0.6933043290881865	0.8761380127652703
0.4485511041434467	0.3066956709118135	0.1238619872347297
0.4485511041434467	0.1933043290881864	0.6238619872347297
0.5514488958565533	0.8066956709118135	0.3761380127652703
0.2172083729973158	0.6892201769663001	0.0452778360981032
0.7827916270026842	0.3107798230336999	0.9547221639018968
0.7827916270026842	0.1892201769663000	0.4547221639018968
0.2172083729973158	0.8107798230336999	0.5452778360981032

Stiffness tensor (GPa):

797.982	113.401	142.431	0.006	17.820	-0.002
113.401	435.462	175.414	-0.033	7.171	-0.020
142.431	175.414	786.561	0.011	19.431	0.003
0.006	-0.033	0.011	269.608	0.005	33.258
17.820	7.171	19.431	0.005	339.312	0.002
-0.002	-0.020	0.003	33.258	0.002	214.392

BN-096

Density (g/cm^3): 3.18 | Space Group: 121
Bulk modulus (GPa): 318 | Shear modulus (GPa): 266
Young's modulus (GPa): 623 | Highest Young's modulus (GPa): 826
Hardness (GPa): 39 | Energy above hull (eV/atom): 0.28

Primitive Cell

1.000000

-2.24007448941924	2.24007448941924	7.74412363137241
2.24007448941924	-2.24007448941924	7.74412363137241
2.24007448941924	2.24007448941924	-7.74412363137241

B N

12 12

DIRECT

0.3835223641078309	0.3835223641078309	0.6663939277237327
0.7171284363840982	0.7171284363840982	0.3336060722762673
0.6164776358921691	0.2828715636159018	0.0000000000000000
0.2828715636159018	0.6164776358921691	0.0000000000000000
0.7022002795540598	0.7022002795540598	0.6581420311910136
0.0440582483630463	0.0440582483630463	0.3418579688089864
0.2977997204459402	0.9559417516369537	0.0000000000000000
0.9559417516369537	0.2977997204459402	0.0000000000000000
0.5346546626603748	0.5346546626603748	0.6510544789310825
0.8836001837292924	0.8836001837292924	0.3489455210689176
0.4653453373396252	0.1163998162707078	0.0000000000000001
0.1163998162707078	0.4653453373396252	0.0000000000000001
0.6378025519671371	0.6378025519671371	0.3759807625437146
0.2618217894234224	0.2618217894234224	0.6240192374562854
0.3621974480328630	0.7381782105765775	0.0000000000000000
0.7381782105765775	0.3621974480328630	0.0000000000000000
0.3114215205201003	0.3114215205201003	0.3692720554974311
0.9421494650226692	0.9421494650226692	0.6307279445025689
0.6885784794798997	0.0578505349773308	0.0000000000000000
0.0578505349773308	0.6885784794798997	0.0000000000000000
0.4775589201328729	0.4775589201328729	0.3735784280581735
0.1039804920746994	0.1039804920746994	0.6264215719418265
0.5224410798671271	0.8960195079253006	0.0000000000000000
0.8960195079253006	0.5224410798671271	0.0000000000000000

Stiffness tensor (GPa):

598.865	143.439	135.185	-0.043	0.003	0.006
143.439	598.861	135.153	-0.002	-0.040	0.025
135.185	135.153	875.525	0.015	0.007	0.019
-0.043	-0.002	0.015	288.647	0.018	0.005
0.003	-0.040	0.007	0.018	288.665	0.005
0.006	0.025	0.019	0.005	0.005	216.360

BN-097

Density (g/cm^3): 3.17 | Space Group: 15

Bulk modulus (GPa): 323 | Shear modulus (GPa): 270

Young's modulus (GPa): 633 | Highest Young's modulus (GPa): 679

Hardness (GPa): 40 | Energy above hull (eV/atom): 0.27

Primitive Cell

1.000000

5.59422359070175	-2.29743207550537	0.00000000000000
5.59422359070175	2.29743207550537	0.00000000000000
-1.71329129734672	0.00000000000000	4.04475601944918

B N

8 8

DIRECT

0.9260188276641406	0.2258533986786155	0.1562910433981315
0.0739811723358594	0.7741466013213845	0.8437089566018685
0.7741466013213845	0.0739811723358594	0.3437089566018685
0.2258533986786155	0.9260188276641406	0.6562910433981315
0.8379530633963810	0.5296368114181560	0.7643896776418038
0.1620469366036191	0.4703631885818441	0.2356103223581962
0.4703631885818441	0.1620469366036191	0.7356103223581962
0.5296368114181560	0.8379530633963810	0.2643896776418038
0.2403072631888563	0.9181879817745491	0.0186494170510834
0.7596927368111437	0.0818120182254510	0.9813505829489166
0.0818120182254510	0.7596927368111437	0.4813505829489166
0.9181879817745491	0.2403072631888563	0.5186494170510834
0.5247935383373985	0.8376246421853475	0.6215346390086878
0.4752064616626015	0.1623753578146525	0.3784653609913122
0.1623753578146525	0.4752064616626015	0.8784653609913122
0.8376246421853477	0.5247935383373985	0.1215346390086878

Stiffness tensor (GPa):

627.751	186.953	182.593	0.003	3.020	0.018
186.953	684.043	80.875	-0.002	31.956	0.023
182.593	80.875	701.078	-0.010	-6.833	0.048
0.003	-0.002	-0.010	282.839	0.014	1.316
3.020	31.956	-6.833	0.014	270.827	-0.013
0.018	0.023	0.048	1.316	-0.013	286.281

BN-098

Density (g/cm^3): 3.17 | Space Group: 41
Bulk modulus (GPa): 313 | Shear modulus (GPa): 279
Young's modulus (GPa): 646 | Highest Young's modulus (GPa): 958
Hardness (GPa): 44 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.85431828049831	0.00000000000000	0.00000000000000
0.00000000000000	3.80270044169062	2.11517211799138
0.00000000000000	-3.80270044169062	2.11517211799138

B N

6 6

DIRECT

0.4058794720739174	0.8546441568484087	0.5155137256604323
0.0941205279260826	0.3546441568484087	0.0155137256604323
0.9058794720739174	0.0155137256604322	0.3546441568484086
0.5941205279260826	0.5155137256604323	0.8546441568484087
0.0000000000000000	0.6648571460008110	0.6648571460008110
0.5000000000000000	0.1648571460008110	0.1648571460008110
0.5810611228979610	0.1440694853583889	0.4883861023089017
0.9189388771020390	0.6440694853583889	0.9883861023089017
0.0810611228979610	0.9883861023089017	0.6440694853583889
0.4189388771020390	0.4883861023089017	0.1440694853583889
0.0000000000000000	0.3325293929353684	0.3325293929353684
0.5000000000000000	0.8325293929353684	0.8325293929353684

Stiffness tensor (GPa):

453.362	194.431	38.534	0.020	0.024	0.000
194.431	851.228	110.482	0.040	0.027	0.025
38.534	110.482	972.982	-0.006	0.040	0.015
0.020	0.040	-0.006	365.707	0.005	0.012
0.024	0.027	0.040	0.005	189.308	-0.004
0.000	0.025	0.015	0.012	-0.004	277.179

BN-099

Density (g/cm^3): 3.15
Space Group: 44
Bulk modulus (GPa): 313
Shear modulus (GPa): 255
Young's modulus (GPa): 602
Highest Young's modulus (GPa): 954
Hardness (GPa): 37
Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

-1.32617127664302	3.49579822041081	2.11625379382444
1.32617127664302	-3.49579822041081	2.11625379382444
1.32617127664302	3.49579822041081	-2.11625379382444

B N

3 3

DIRECT

0.3394325632428786	0.8394325632428785	0.5000000000000000
0.6209977395019928	0.3139925021106240	0.3070052373913688
0.0069872647192553	0.3139925021106240	0.6929947626086312
0.6673340224292205	0.1673340224292205	0.5000000000000000
0.3741574529496616	0.6826242079776830	0.6915332449719787
0.9910909630057043	0.6826242079776830	0.3084667550280213

Stiffness tensor (GPa):

577.428	57.397	20.668	-0.022	0.010	0.006
57.397	957.420	131.395	0.019	-0.036	0.013
20.668	131.395	972.527	-0.012	-0.007	0.008
-0.022	0.019	-0.012	389.725	0.013	-0.003
0.010	-0.036	-0.007	0.013	138.188	0.001
0.006	0.013	0.008	-0.003	0.001	141.276

BN-100

Density (g/cm^3): 3.13 | Space Group: 88
Bulk modulus (GPa): 250 | Shear modulus (GPa): 208
Young's modulus (GPa): 489 | Highest Young's modulus (GPa): 570
Hardness (GPa): 34 | Energy above hull (eV/atom): 0.79

Primitive Cell

1.000000

-3.97930201181553	3.97930201181553	3.32480295669318
3.97930201181553	-3.97930201181553	3.32480295669318
3.97930201181553	3.97930201181553	-3.32480295669318

B N

16 16

DIRECT

0.8769972351264488	0.2125755639191262	0.1373543447639422
0.8730027648735512	0.0374244360808738	0.3626456552360579
0.0752212191551840	0.7396428903625066	0.8626456552360577
0.6747787808448159	0.5103571096374934	0.6373543447639421
0.9625755639191262	0.3252212191551841	0.8355783287926775
0.7874244360808738	0.9247787808448160	0.6644216712073225
0.4896428903625066	0.1269972351264488	0.1644216712073225
0.2603571096374934	0.1230027648735512	0.3355783287926773
0.0550448765232661	0.7503452141973317	0.5262293938555849
0.6949551234767339	0.4996547858026683	0.9737706061444151
0.2241158203417468	0.5288154826676812	0.4737706061444151
0.5258841796582532	0.7211845173323188	0.0262293938555849
0.2788154826676812	0.3050448765232661	0.8046996623259344
0.4711845173323188	0.9449551234767339	0.6953003376740656
0.5003452141973317	0.4741158203417468	0.1953003376740657
0.2496547858026683	0.7758841796582532	0.3046996623259344
0.6523130967756908	0.0252239636377172	0.1761248319705974
0.0976869032243091	0.2247760363622828	0.3238751680294026
0.8490991316671198	0.4761882648050935	0.8238751680294026
0.9009008683328802	0.7738117351949065	0.6761248319705974
0.2261882648050935	0.9023130967756908	0.1270891331379737
0.5238117351949065	0.3476869032243092	0.3729108668620263
0.7752239636377172	0.0990991316671198	0.8729108668620262
0.9747760363622828	0.1509008683328802	0.6270891331379737
0.5138331490487775	0.5287324754488542	0.7887174015001308
0.2361668509512226	0.7212675245511460	0.7112825984998692
0.7400150739487235	0.7251157475486467	0.2112825984998693
0.0099849260512766	0.5248842524513533	0.2887174015001308
0.2787324754488542	0.9900150739487235	0.5148993264000767
0.4712675245511460	0.2599849260512767	0.9851006735999234
0.4751157475486467	0.7638331490487775	0.4851006735999233
0.2748842524513533	0.4861668509512226	0.0148993264000767

Stiffness tensor (GPa):

441.667	172.649	117.271	-0.005	0.003	-7.232
172.649	441.690	117.278	0.004	0.022	7.244
117.271	117.278	554.294	-0.004	-0.011	0.008
-0.005	0.004	-0.004	221.389	0.012	0.015
0.003	0.022	-0.011	0.012	221.391	-0.001
-7.232	7.244	0.008	0.015	-0.001	287.571

BN-101

Density (g/cm^3): 3.13 | Space Group: 108

Bulk modulus (GPa): 330 | Shear modulus (GPa): 278

Young's modulus (GPa): 652 | Highest Young's modulus (GPa): 952

Hardness (GPa): 41 | Energy above hull (eV/atom): 0.24

Primitive Cell

1.000000

-2.49870820653686	2.49870820653686	2.10976176084739
2.49870820653686	-2.49870820653686	2.10976176084739
2.49870820653686	2.49870820653686	-2.10976176084739

B N

4 4

DIRECT

0.5389695222112547	0.3296468037126770	0.5000000000000000
0.8296468037126770	0.0389695222112547	0.5000000000000000
0.0389695222112547	0.5389695222112547	0.2093227184985778
0.3296468037126770	0.8296468037126770	0.7906772815014222
0.4721331520198393	0.6592505220165989	0.5000000000000000
0.1592505220165989	0.9721331520198393	0.5000000000000000
0.9721331520198393	0.4721331520198393	0.8128826300032403
0.6592505220165989	0.1592505220165989	0.1871173699967597

Stiffness tensor (GPa):

582.612	312.733	57.198	0.029	-0.000	0.030
312.733	582.621	57.221	-0.004	0.027	0.038
57.198	57.221	959.170	0.013	0.018	0.052
0.029	-0.004	0.013	288.302	0.004	-0.006
-0.000	0.027	0.018	0.004	288.308	0.004
0.030	0.038	0.052	-0.006	0.004	357.156

BN-102

Density (g/cm^3): 3.13 | Space Group: 114
Bulk modulus (GPa): 300 | Shear modulus (GPa): 245
Young's modulus (GPa): 578 | Highest Young's modulus (GPa): 716
Hardness (GPa): 36 | Energy above hull (eV/atom): 0.27

Primitive Cell

1.000000

4.55141292857274	0.00000000000000	0.00000000000000
0.00000000000000	4.55141292857274	0.00000000000000
0.00000000000000	0.00000000000000	10.18251253644261

B N

16 16

DIRECT

0.8396748384338876	0.8301123796998222	0.6935981038673724
0.1603251615661124	0.1698876203001778	0.6935981038673724
0.8301123796998222	0.1603251615661124	0.3064018961326276
0.1698876203001778	0.8396748384338876	0.3064018961326276
0.3396748384338877	0.6698876203001778	0.8064018961326276
0.6603251615661124	0.3301123796998222	0.8064018961326276
0.3301123796998222	0.3396748384338877	0.1935981038673724
0.6698876203001778	0.6603251615661124	0.1935981038673724
0.1657414409606647	0.6674837210347144	0.0566129624726548
0.8342585590393353	0.3325162789652856	0.0566129624726548
0.6674837210347144	0.8342585590393353	0.9433870375273452
0.3325162789652856	0.1657414409606647	0.9433870375273452
0.6657414409606647	0.8325162789652856	0.4433870375273452
0.3342585590393353	0.1674837210347144	0.4433870375273452
0.1674837210347144	0.6657414409606647	0.5566129624726548
0.8325162789652856	0.3342585590393353	0.5566129624726548
0.6956105629042062	0.6752520973688165	0.8071349504628138
0.3043894370957938	0.3247479026311835	0.8071349504628138
0.6752520973688165	0.3043894370957938	0.1928650495371862
0.3247479026311835	0.6956105629042062	0.1928650495371862
0.1956105629042062	0.8247479026311835	0.6928650495371862
0.8043894370957938	0.1752520973688165	0.6928650495371862
0.1752520973688165	0.1956105629042062	0.3071349504628138
0.8247479026311835	0.8043894370957938	0.3071349504628138
0.3212368536779756	0.8116002119259196	0.4429360210309102
0.6787631463220244	0.1883997880740804	0.4429360210309102
0.8116002119259196	0.6787631463220244	0.5570639789690898
0.1883997880740804	0.3212368536779756	0.5570639789690898
0.8212368536779756	0.6883997880740804	0.0570639789690898
0.1787631463220244	0.3116002119259196	0.0570639789690898
0.3116002119259196	0.8212368536779756	0.9429360210309102
0.6883997880740804	0.1787631463220244	0.9429360210309102

Stiffness tensor (GPa):

549.803	124.231	152.164	0.001	0.028	0.007
124.231	549.779	152.122	-0.007	0.016	0.011
152.164	152.122	784.231	0.012	0.001	0.041
0.001	-0.007	0.012	278.186	0.014	0.002
0.028	0.016	0.001	0.014	278.204	0.005
0.007	0.011	0.041	0.002	0.005	199.914

BN-103

Density (g/cm^3): 3.12 | Space Group: 88
Bulk modulus (GPa): 253 | Shear modulus (GPa): 217
Young's modulus (GPa): 506 | Highest Young's modulus (GPa): 619
Hardness (GPa): 36 | Energy above hull (eV/atom): 0.61

Primitive Cell

1.000000

-3.99006539325470	3.99006539325470	3.31801009015300
3.99006539325470	-3.99006539325470	3.31801009015300
3.99006539325470	3.99006539325470	-3.31801009015300

B N

16 16

DIRECT

0.6089052374949995	0.4243610925761290	0.3742544549032596
0.1410947625050005	0.8256389074238710	0.1257455450967404
0.0501066376728694	0.2346507825917399	0.6257455450967404
0.6998933623271306	0.0153492174082601	0.8742544549032596
0.9846507825917399	0.8589052374949995	0.6845441449188705
0.7653492174082601	0.3910947625050005	0.8154558550811295
0.1743610925761290	0.3001066376728694	0.3154558550811295
0.5756389074238710	0.9498933623271306	0.1845441449188705
0.1847164471444784	0.4713545540150668	0.0784810402762091
0.5652835528555216	0.7786454459849332	0.4215189597237909
0.3928735137388577	0.1062354068682694	0.9215189597237909
0.3571264862611423	0.1437645931317306	0.5784810402762091
0.8562354068682694	0.4347164471444784	0.2133618931294117
0.8937645931317306	0.8152835528555216	0.2866381068705883
0.2213545540150668	0.6428735137388577	0.7866381068705883
0.5286454459849332	0.6071264862611423	0.7133618931294117
0.7212521306716581	0.8437048032001261	0.6846981985079417
0.0287478693283420	0.4062951967998740	0.8153018014920583
0.1590066046921844	0.0365539321637163	0.3153018014920583
0.5909933953078156	0.2134460678362836	0.1846981985079417
0.5937048032001260	0.4090066046921843	0.6224526725284680
0.1562951967998739	0.8409933953078156	0.8775473274715320
0.7865539321637163	0.9712521306716579	0.3775473274715320
0.9634460678362837	0.2787478693283420	0.1224526725284680
0.3387806569810681	0.7743045889320606	0.2292782407958248
0.4112193430189318	0.4756954110679394	0.2707217592041752
0.5450263481362358	0.1095024161852434	0.7707217592041753
0.2049736518637642	0.1404975838147566	0.7292782407958247
0.5243045889320606	0.7950263481362358	0.9355239319509925
0.2256954110679395	0.4549736518637642	0.5644760680490075
0.8595024161852434	0.5887806569810681	0.0644760680490076
0.8904975838147566	0.6612193430189318	0.4355239319509924

Stiffness tensor (GPa):

538.774	144.282	68.563	0.008	0.020	25.724
144.282	538.745	68.549	-0.015	0.010	-25.700
68.563	68.549	632.940	-0.004	0.000	0.036
0.008	-0.015	-0.004	227.167	-0.001	0.006
0.020	0.010	0.000	-0.001	227.136	0.005
25.724	-25.700	0.036	0.006	0.005	173.405

BN-104

Density (g/cm^3): 3.11 | Space Group: 62

Bulk modulus (GPa): 303 | Shear modulus (GPa): 232

Young's modulus (GPa): 555 | Highest Young's modulus (GPa): 860

Hardness (GPa): 33 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

5.21916048933558	0.00000000000000	0.00000000000000
0.00000000000000	6.97800069279169	0.00000000000000
0.00000000000000	0.00000000000000	4.36785119577434

B N

12 12

DIRECT

0.3684266701457132	0.5596136138324743	0.8222656515983133
0.6315733298542867	0.4403863861675256	0.1777343484016866
0.6315733298542867	0.0596136138324743	0.1777343484016866
0.3684266701457132	0.9403863861675258	0.8222656515983133
0.3722588864370781	0.7500000000000001	0.3436767033139276
0.6277411135629218	0.2499999999999999	0.6563232966860724
0.8684266701457133	0.9403863861675258	0.6777343484016867
0.1315733298542867	0.0596136138324743	0.3222656515983133
0.1315733298542867	0.4403863861675256	0.3222656515983133
0.8684266701457133	0.5596136138324743	0.6777343484016867
0.8722588864370782	0.7500000000000001	0.1563232966860723
0.1277411135629218	0.2499999999999999	0.8436767033139276
0.3579840779003093	0.9372546594190221	0.1812017554322154
0.6420159220996906	0.0627453405809779	0.8187982445677846
0.6420159220996906	0.4372546594190219	0.8187982445677846
0.3579840779003093	0.5627453405809781	0.1812017554322154
0.3829926618374555	0.7500000000000001	0.6623817019704330
0.6170073381625445	0.2499999999999999	0.3376182980295669
0.8579840779003094	0.5627453405809781	0.3187982445677845
0.1420159220996906	0.4372546594190219	0.6812017554322154
0.1420159220996906	0.0627453405809779	0.6812017554322154
0.8579840779003094	0.9372546594190221	0.3187982445677845
0.8829926618374555	0.7500000000000001	0.8376182980295670
0.1170073381625445	0.2499999999999999	0.1623817019704330

Stiffness tensor (GPa):

465.505	75.009	94.116	-0.001	-0.001	0.019
75.009	876.584	174.303	0.012	-0.003	-0.008
94.116	174.303	839.026	-0.010	-0.003	0.026
-0.001	0.012	-0.010	374.757	0.019	0.014
-0.001	-0.003	-0.003	0.019	154.229	-0.007
0.019	-0.008	0.026	0.014	-0.007	131.238

BN-105

Density (g/cm^3): 3.11 | Space Group: 187
Bulk modulus (GPa): 301 | Shear modulus (GPa): 244
Young's modulus (GPa): 577 | Highest Young's modulus (GPa): 939
Hardness (GPa): 36 | Energy above hull (eV/atom): 0.34

Primitive Cell

1.000000

7.21417890686008	0.00000000000000	0.00000000000000
-3.60708945343004	6.24766220078668	0.00000000000000
0.00000000000000	0.00000000000000	2.64977861657233

B N

9 9

DIRECT

0.2523329496224671	0.1261664748112335	0.0000000000000000
0.8738335251887664	0.1261664748112335	0.0000000000000000
0.8738335251887664	0.7476670503775329	0.0000000000000000
0.8957624264113999	0.4478812132056998	0.5000000000000000
0.5521187867943000	0.4478812132056998	0.5000000000000000
0.5521187867943000	0.1042375735886001	0.5000000000000000
0.5812886433407558	0.7906443216703780	0.5000000000000000
0.2093556783296221	0.7906443216703780	0.5000000000000000
0.2093556783296220	0.4187113566592441	0.5000000000000000
0.7478404926522377	0.8739202463261189	0.0000000000000000
0.1260797536738812	0.8739202463261189	0.0000000000000000
0.1260797536738811	0.2521595073477622	0.0000000000000000
0.1103353775044726	0.5551676887522364	0.5000000000000000
0.4448323112477637	0.5551676887522363	0.5000000000000000
0.4448323112477638	0.8896646224955275	0.5000000000000000
0.4194944259178612	0.2097472129589306	0.5000000000000000
0.7902527870410694	0.2097472129589306	0.5000000000000000
0.7902527870410694	0.5805055740821389	0.5000000000000000

Stiffness tensor (GPa):

966.734	164.693	10.768	-0.008	0.023	0.054
164.693	966.658	10.837	0.033	0.026	0.026
10.768	10.837	552.196	0.000	0.023	0.032
-0.008	0.033	0.000	123.105	0.003	0.005
0.023	0.026	0.023	0.003	123.010	-0.018
0.054	0.026	0.032	0.005	-0.018	400.634

BN-106

Density (g/cm^3): 3.10 | Space Group: 121
Bulk modulus (GPa): 299 | Shear modulus (GPa): 246
Young's modulus (GPa): 579 | Highest Young's modulus (GPa): 763
Hardness (GPa): 37 | Energy above hull (eV/atom): 0.35

Primitive Cell

1.000000

-2.26359664081266	2.26359664081266	5.18841187999959
2.26359664081266	-2.26359664081266	5.18841187999959
2.26359664081266	2.26359664081266	-5.18841187999959

B	N
8	8

DIRECT

0.0173705411890122	0.0173705411890122	0.6583208807226995
0.3590496604663127	0.3590496604663127	0.3416791192773005
0.9826294588109878	0.6409503395336873	0.0000000000000000
0.6409503395336873	0.9826294588109878	0.0000000000000000
0.2587169196149424	0.2587169196149424	0.6673344326270332
0.5913824869879092	0.5913824869879092	0.3326655673729668
0.7412830803850576	0.4086175130120908	0.0000000000000000
0.4086175130120908	0.7412830803850576	0.0000000000000000
0.9961747646627307	0.9961747646627307	0.3682804337661005
0.6278943308966300	0.6278943308966300	0.6317195662338994
0.0038252353372693	0.3721056691033698	0.0000000000000001
0.3721056691033698	0.0038252353372693	0.0000000000000001
0.7614830367077867	0.7614830367077867	0.3726746553998832
0.3888083813079035	0.3888083813079035	0.6273253446001168
0.2385169632922133	0.6111916186920965	0.0000000000000000
0.6111916186920965	0.2385169632922133	0.0000000000000000

Stiffness tensor (GPa):

536.425	131.562	145.285	0.057	0.017	-0.004
131.562	536.460	145.317	-0.010	0.055	0.014
145.285	145.317	826.601	0.002	-0.012	0.007
0.057	-0.010	0.002	275.929	-0.033	0.006
0.017	0.055	-0.012	-0.033	275.926	0.001
-0.004	0.014	0.007	0.006	0.001	204.984

BN-107

Density (g/cm^3): 3.08 | Space Group: 60

Bulk modulus (GPa): 292 | Shear modulus (GPa): 230

Young's modulus (GPa): 546 | Highest Young's modulus (GPa): 696

Hardness (GPa): 33 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.79443569253077	0.00000000000000	0.00000000000000
0.00000000000000	5.03579795878242	0.00000000000000
0.00000000000000	0.00000000000000	4.44006156025590

B N

8 8

DIRECT

0.1592301797547759	0.6391422672242233	0.0785525962317770
0.8407698202452241	0.3608577327757767	0.9214474037682230
0.8407698202452241	0.6391422672242233	0.4214474037682231
0.1592301797547759	0.3608577327757767	0.5785525962317769
0.3407698202452241	0.8608577327757766	0.5785525962317769
0.6592301797547759	0.1391422672242233	0.4214474037682231
0.6592301797547759	0.8608577327757766	0.9214474037682230
0.3407698202452241	0.1391422672242233	0.0785525962317770
0.8148764363466421	0.3616711399482367	0.5723030464938591
0.1851235636533579	0.6383288600517634	0.4276969535061409
0.1851235636533579	0.3616711399482367	0.9276969535061408
0.8148764363466421	0.6383288600517634	0.0723030464938592
0.6851235636533579	0.1383288600517634	0.0723030464938592
0.3148764363466421	0.8616711399482366	0.9276969535061408
0.3148764363466421	0.1383288600517634	0.4276969535061409
0.6851235636533579	0.8616711399482366	0.5723030464938591

Stiffness tensor (GPa):

340.955	209.457	136.216	0.005	0.003	0.018
209.457	736.767	131.776	0.012	-0.003	0.027
136.216	131.776	754.084	-0.012	-0.003	0.038
0.005	0.012	-0.012	311.305	-0.002	0.012
0.003	-0.003	-0.003	-0.002	205.348	0.001
0.018	0.027	0.038	0.012	0.001	253.365

BN-108

Density (g/cm^3): 3.07	Space Group: 62
Bulk modulus (GPa): 302	Shear modulus (GPa): 219
Young's modulus (GPa): 530	Highest Young's modulus (GPa): 750
Hardness (GPa): 29	Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

4.85623351404506	0.00000000000000	0.00000000000000
0.00000000000000	2.58537653375610	0.00000000000000
0.00000000000000	0.00000000000000	4.28295966713537

B N

4 4

DIRECT

0.1599119800371231	0.7500000000000000	0.5914934680461568
0.8400880199628769	0.2500000000000001	0.4085065319538432
0.3400880199628769	0.2500000000000001	0.0914934680461568
0.6599119800371231	0.7500000000000000	0.9085065319538432
0.8215287024585485	0.7500000000000000	0.6082383540977019
0.1784712975414515	0.2500000000000001	0.3917616459022981
0.6784712975414515	0.2500000000000001	0.1082383540977019
0.3215287024585485	0.7500000000000000	0.8917616459022981

Stiffness tensor (GPa):

367.408	107.754	280.998	-0.003	0.008	0.006
107.754	784.519	120.139	-0.003	0.003	-0.002
280.998	120.139	679.075	-0.004	-0.045	-0.015
-0.003	-0.003	-0.004	300.248	-0.016	0.003
0.008	0.003	-0.045	-0.016	273.821	0.002
0.006	-0.002	-0.015	0.003	0.002	184.740

BN-109

Density (g/cm^3): 3.03 | Space Group: 62
Bulk modulus (GPa): 312 | Shear modulus (GPa): 219
Young's modulus (GPa): 533 | Highest Young's modulus (GPa): 755
Hardness (GPa): 28 | Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

6.47889348084760	0.00000000000000	0.00000000000000
0.00000000000000	2.57872345191131	0.00000000000000
0.00000000000000	0.00000000000000	6.50455189873503

B N

8 8

DIRECT

0.8771724934515759	0.7500000000000000	0.9444896964153353
0.3771724934515759	0.7500000000000000	0.5555103035846647
0.1228275065484241	0.2500000000000000	0.0555103035846647
0.6228275065484241	0.2500000000000000	0.4444896964153353
0.4653717385705023	0.7500000000000000	0.1285201577980457
0.9653717385705023	0.7500000000000000	0.3714798422019543
0.5346282614294977	0.2500000000000000	0.8714798422019543
0.0346282614294977	0.2500000000000000	0.6285201577980457
0.1432922311616617	0.7500000000000000	0.5493050932662427
0.6432922311616617	0.7500000000000000	0.9506949067337573
0.8567077688383383	0.2500000000000000	0.4506949067337573
0.3567077688383383	0.2500000000000000	0.0493050932662427
0.5249222438613144	0.7500000000000000	0.3521620313242785
0.0249222438613144	0.7500000000000000	0.1478379686757215
0.4750777561386856	0.2500000000000000	0.6478379686757215
0.9750777561386856	0.2500000000000000	0.8521620313242785

Stiffness tensor (GPa):

712.568	95.813	139.813	0.000	0.007	0.017
95.813	778.228	100.445	0.009	-0.005	0.015
139.813	100.445	650.589	0.004	-0.010	0.013
0.000	0.009	0.004	223.733	-0.002	0.000
0.007	-0.005	-0.010	-0.002	101.324	0.003
0.017	0.015	0.013	0.000	0.003	261.023

BN-110

Density (g/cm^3): 3.03 | Space Group: 94
Bulk modulus (GPa): 279 | Shear modulus (GPa): 220
Young's modulus (GPa): 523 | Highest Young's modulus (GPa): 667
Hardness (GPa): 33 | Energy above hull (eV/atom): 0.36

Primitive Cell

1.000000

4.60731467444709	0.00000000000000	0.00000000000000
0.00000000000000	4.60731467444709	0.00000000000000
0.00000000000000	0.00000000000000	7.68583843743684

B N

12 12

DIRECT

0.3398558466959313	0.6601441533040686	0.5000000000000000
0.6601441533040686	0.3398558466959314	0.5000000000000000
0.8398558466959314	0.8398558466959314	0.0000000000000000
0.1601441533040686	0.1601441533040687	0.0000000000000000
0.8368419646579541	0.6643702741346745	0.3247849703086937
0.1631580353420459	0.3356297258653255	0.3247849703086937
0.8356297258653255	0.3368419646579541	0.8247849703086937
0.1643702741346744	0.6631580353420459	0.8247849703086937
0.6631580353420459	0.1643702741346744	0.1752150296913063
0.3368419646579541	0.8356297258653255	0.1752150296913063
0.6643702741346745	0.8368419646579541	0.6752150296913063
0.3356297258653255	0.1631580353420459	0.6752150296913063
0.1838098248381417	0.8161901751618583	0.0000000000000000
0.8161901751618583	0.1838098248381417	0.0000000000000000
0.6838098248381417	0.6838098248381417	0.5000000000000000
0.3161901751618583	0.3161901751618583	0.5000000000000000
0.6762293355215714	0.8038107562721811	0.1745677510430148
0.3237706644784286	0.1961892437278189	0.1745677510430148
0.6961892437278189	0.1762293355215714	0.6745677510430148
0.3038107562721812	0.8237706644784286	0.6745677510430148
0.8237706644784286	0.3038107562721812	0.3254322489569852
0.1762293355215714	0.6961892437278189	0.3254322489569852
0.8038107562721811	0.6762293355215714	0.8254322489569852
0.1961892437278189	0.3237706644784286	0.8254322489569852

Stiffness tensor (GPa):

478.230	120.006	157.248	-0.021	0.005	0.025
120.006	478.226	157.220	0.010	0.017	-0.014
157.248	157.220	747.697	0.035	-0.032	0.020
-0.021	0.010	0.035	271.501	0.007	0.009
0.005	0.017	-0.032	0.007	271.507	-0.006
0.025	-0.014	0.020	0.009	-0.006	165.074

BN-111

Density (g/cm^3): 3.02 | Space Group: 81
Bulk modulus (GPa): 286 | Shear modulus (GPa): 220
Young's modulus (GPa): 525 | Highest Young's modulus (GPa): 623
Hardness (GPa): 32 | Energy above hull (eV/atom): 0.34

Primitive Cell

1.000000

4.62508184562961	0.00000000000000	0.00000000000000
0.00000000000000	4.62508184562961	0.00000000000000
0.00000000000000	0.00000000000000	7.65607800771247

B N

12 12

DIRECT

0.1590580858975754	0.1679883910591113	0.2435213019001483
0.8409419141024246	0.8320116089408887	0.2435213019001483
0.1679883910591113	0.8409419141024246	0.7564786980998517
0.8320116089408887	0.1590580858975754	0.7564786980998517
0.8345920579147696	0.3341401818222165	0.4255841199271106
0.1654079420852304	0.6658598181777835	0.4255841199271106
0.6658598181777835	0.8345920579147696	0.5744158800728894
0.3341401818222165	0.1654079420852304	0.5744158800728894
0.6561550032352437	0.3323087893453225	0.1022405062815443
0.3438449967647563	0.6676912106546775	0.1022405062815443
0.6676912106546775	0.6561550032352437	0.8977594937184556
0.3323087893453225	0.3438449967647563	0.8977594937184556
0.8110734286558903	0.1729082857416826	0.2428449003329813
0.1889265713441097	0.8270917142583174	0.2428449003329813
0.8270917142583174	0.8110734286558903	0.7571550996670187
0.1729082857416826	0.1889265713441097	0.7571550996670187
0.1851161424904995	0.3221567992498235	0.4263475007603578
0.8148838575095005	0.6778432007501765	0.4263475007603578
0.3221567992498235	0.8148838575095005	0.5736524992396421
0.6778432007501765	0.1851161424904995	0.5736524992396421
0.3121374408959698	0.3242974685758968	0.1027454028647414
0.6878625591040302	0.6757025314241032	0.1027454028647414
0.3242974685758968	0.6878625591040302	0.8972545971352586
0.6757025314241032	0.3121374408959698	0.8972545971352586

Stiffness tensor (GPa):

481.767	127.922	175.080	-0.043	-0.016	6.450
127.922	481.774	175.063	0.023	-0.036	-6.462
175.080	175.063	705.562	-0.003	0.015	0.003
-0.043	0.023	-0.003	261.337	0.062	-0.004
-0.016	-0.036	0.015	0.062	261.407	-0.006
6.450	-6.462	0.003	-0.004	-0.006	199.048

BN-112

Density (g/cm^3): 3.02 Space Group: 130

Bulk modulus (GPa): 312 Shear modulus (GPa): 226

Young's modulus (GPa): 547 Highest Young's modulus (GPa): 652

Hardness (GPa): 30 Energy above hull (eV/atom): 0.29

Primitive Cell

1.000000

7.04128365135594	0.00000000000000	0.00000000000000
0.00000000000000	7.04128365135594	0.00000000000000
0.00000000000000	0.00000000000000	4.40873287976532

B N

16 16

DIRECT

0.2419926367753413	0.3976156937741457	0.4183316898441781
0.7580073632246587	0.6023843062258543	0.4183316898441781
0.3976156937741457	0.7580073632246587	0.5816683101558219
0.6023843062258543	0.2419926367753413	0.5816683101558219
0.2419926367753413	0.6023843062258543	0.9183316898441781
0.7580073632246587	0.3976156937741457	0.9183316898441781
0.3976156937741457	0.2419926367753413	0.0816683101558219
0.6023843062258543	0.7580073632246587	0.0816683101558219
0.2580073632246586	0.1023843062258542	0.5816683101558219
0.7419926367753413	0.8976156937741457	0.5816683101558219
0.1023843062258542	0.7419926367753413	0.4183316898441781
0.8976156937741457	0.2580073632246586	0.4183316898441781
0.2580073632246586	0.8976156937741457	0.0816683101558219
0.7419926367753413	0.1023843062258542	0.0816683101558219
0.1023843062258542	0.2580073632246586	0.9183316898441781
0.8976156937741457	0.7419926367753413	0.9183316898441781
0.7576804767184548	0.5911665180813188	0.0627022827287908
0.2423195232815451	0.4088334819186812	0.0627022827287908
0.5911665180813188	0.2423195232815451	0.9372977172712091
0.4088334819186812	0.7576804767184548	0.9372977172712091
0.7576804767184548	0.4088334819186812	0.5627022827287909
0.2423195232815451	0.5911665180813188	0.5627022827287909
0.5911665180813188	0.7576804767184548	0.4372977172712092
0.4088334819186812	0.2423195232815451	0.4372977172712092
0.7423195232815452	0.9088334819186813	0.9372977172712091
0.2576804767184548	0.0911665180813186	0.9372977172712091
0.9088334819186813	0.2576804767184548	0.0627022827287908
0.0911665180813186	0.7423195232815452	0.0627022827287908
0.7423195232815452	0.0911665180813186	0.4372977172712092
0.2576804767184548	0.9088334819186813	0.4372977172712092
0.9088334819186813	0.7423195232815452	0.5627022827287909
0.0911665180813186	0.2576804767184548	0.5627022827287909

Stiffness tensor (GPa):

678.456	130.061	124.880	-0.005	-0.000	0.004
130.061	678.487	124.944	0.033	0.001	0.023
124.880	124.944	690.741	-0.024	0.002	0.034
-0.005	0.033	-0.024	252.498	0.009	0.009
-0.000	0.001	0.002	0.009	252.555	-0.009
0.004	0.023	0.034	0.009	-0.009	123.919

BN-113

Density (g/cm^3): 3.01 | Space Group: 36
Bulk modulus (GPa): 305 | Shear modulus (GPa): 227
Young's modulus (GPa): 546 | Highest Young's modulus (GPa): 713
Hardness (GPa): 31 | Energy above hull (eV/atom): 0.33

Primitive Cell

1.000000

3.54879902458334	-2.19712389568061	0.00000000000000
3.54879902458334	2.19712389568061	0.00000000000000
0.00000000000000	0.00000000000000	7.03077068291748

B N

8 8

DIRECT

0.1704768697560735	0.8295231302439265	0.1178658709670131
0.8295231302439265	0.1704768697560735	0.6178658709670133
0.3366156544189263	0.6633843455810737	0.8223381821327832
0.6633843455810737	0.3366156544189263	0.3223381821327833
0.4772517245803812	0.8210464827928876	0.4810523964117899
0.5227482754196189	0.1789535172071124	0.9810523964117900
0.8210464827928876	0.4772517245803812	0.9810523964117900
0.1789535172071124	0.5227482754196189	0.4810523964117899
0.1887221672808060	0.8112778327191941	0.6295442324680101
0.8112778327191941	0.1887221672808060	0.1295442324680098
0.3115638681654609	0.6884361318345391	0.3122154870778504
0.6884361318345391	0.3115638681654609	0.8122154870778504
0.4687386040830159	0.8493951870883258	0.9831907264996502
0.5312613959169842	0.1506048129116740	0.4831907264996501
0.8493951870883260	0.4687386040830158	0.4831907264996501
0.1506048129116741	0.5312613959169841	0.9831907264996502

Stiffness tensor (GPa):

740.986	95.752	113.843	-0.025	0.013	0.029
95.752	659.905	123.602	0.005	-0.000	0.024
113.843	123.602	679.840	-0.025	-0.008	0.051
-0.025	0.005	-0.025	231.178	0.033	-0.002
0.013	-0.000	-0.008	0.033	125.269	0.004
0.029	0.024	0.051	-0.002	0.004	252.034

BN-114

Density (g/cm^3): 2.98 | Space Group: 87

Bulk modulus (GPa): 280 | Shear modulus (GPa): 230

Young's modulus (GPa): 542 | Highest Young's modulus (GPa): 961

Hardness (GPa): 35 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

-4.67961718445379	4.67961718445379	1.26214403373624
4.67961718445379	-4.67961718445379	1.26214403373624
4.67961718445379	4.67961718445379	-1.26214403373624

B N

8 8

DIRECT

0.8059055499687056	0.1383066336601983	0.9442121836289039
0.1940944500312944	0.8616933663398016	0.0557878163710961
0.8616933663398016	0.8059055499687056	0.6675989163085072
0.1383066336601984	0.1940944500312944	0.3324010836914928
0.8256772691530643	0.5484543090078084	0.3741315781608727
0.1743227308469357	0.4515456909921916	0.6258684218391273
0.5484543090078084	0.1743227308469357	0.7227770398547442
0.4515456909921916	0.8256772691530643	0.2772229601452558
0.6836557373259022	0.6340008251810001	0.3176565625069022
0.3163442626740978	0.3659991748190001	0.6823434374930979
0.6340008251809999	0.3163442626740978	0.9503450878550976
0.3659991748190001	0.6836557373259022	0.0496549121449023
0.6688090712238739	0.0477359765283727	0.7165450477522466
0.3311909287761263	0.9522640234716273	0.2834549522477535
0.9522640234716273	0.6688090712238739	0.6210730946955012
0.0477359765283727	0.3311909287761262	0.3789269053044989

Stiffness tensor (GPa):

440.079	202.701	81.677	0.006	0.038	-2.979
202.701	440.129	81.721	0.012	-0.016	2.940
81.677	81.721	981.715	0.016	-0.009	-0.044
0.006	0.012	0.016	253.121	-0.002	0.018
0.038	-0.016	-0.009	-0.002	253.084	-0.005
-2.979	2.940	-0.044	0.018	-0.005	232.440

BN-115

Density (g/cm^3): 2.97 Space Group: 87

Bulk modulus (GPa): 299 Shear modulus (GPa): 207

Young's modulus (GPa): 504 Highest Young's modulus (GPa): 737

Hardness (GPa): 26 Energy above hull (eV/atom): 0.33

Primitive Cell

1.000000

-3.28302514426153	3.28302514426153	1.28592990088970
3.28302514426153	-3.28302514426153	1.28592990088970
3.28302514426153	3.28302514426153	-1.28592990088970

B N

4 4

DIRECT

0.2921066135275951	0.8741230196273702	0.1662296331549653
0.7078933864724049	0.1258769803726298	0.8337703668450347
0.1258769803726298	0.2921066135275951	0.4179835939002250
0.8741230196273702	0.7078933864724049	0.5820164060997750
0.7172208636617623	0.8945891979613252	0.6118100616230875
0.2827791363382377	0.1054108020386748	0.3881899383769125
0.8945891979613252	0.2827791363382377	0.1773683342995629
0.1054108020386748	0.7172208636617623	0.8226316657004371

Stiffness tensor (GPa):

626.428	192.809	74.823	-0.015	0.006	4.578
192.809	626.409	74.854	-0.006	0.009	-4.557
74.823	74.854	750.307	0.008	0.004	0.042
-0.015	-0.006	0.008	240.758	-0.006	-0.001
0.006	0.009	0.004	-0.006	240.728	-0.000
4.578	-4.557	0.042	-0.001	-0.000	93.604

BN-116

Density (g/cm^3): 2.95 | Space Group: 71

Bulk modulus (GPa): 287 | Shear modulus (GPa): 191

Young's modulus (GPa): 470 | Highest Young's modulus (GPa): 904

Hardness (GPa): 24 | Energy above hull (eV/atom): 0.17

Primitive Cell

1.000000

-1.26758653576183	3.10586567973230	5.32672294581604
1.26758653576183	-3.10586567973230	5.32672294581604
1.26758653576183	3.10586567973230	-5.32672294581604

B N

6 6

DIRECT

0.6881374333458761	0.6881374333458761	0.0000000000000000
0.3118625666541239	0.3118625666541239	0.0000000000000000
0.3233756337075722	0.0000000000000000	0.3233756337075722
0.6766243662924278	0.0000000000000000	0.6766243662924278
0.8940429040194240	0.3940429040194240	0.5000000000000000
0.1059570959805760	0.6059570959805760	0.5000000000000000
0.1817818487174532	0.1817818487174531	0.0000000000000000
0.8182181512825468	0.8182181512825468	0.0000000000000000
0.8109255055014681	0.5000000000000000	0.3109255055014681
0.1890744944985319	0.5000000000000000	0.6890744944985319
0.3870003065082466	0.8870003065082466	0.5000000000000000
0.6129996934917534	0.1129996934917534	0.5000000000000000

Stiffness tensor (GPa):

935.375	58.415	146.742	-0.010	0.009	0.005
58.415	398.495	128.050	0.011	0.035	0.027
146.742	128.050	767.620	0.008	0.040	0.034
-0.010	0.011	0.008	61.407	0.021	0.001
0.009	0.035	0.040	0.021	336.028	0.001
0.005	0.027	0.034	0.001	0.001	169.883

BN-117

Density (g/cm^3): 2.94 | Space Group: 138
Bulk modulus (GPa): 283 | Shear modulus (GPa): 207
Young's modulus (GPa): 500 | Highest Young's modulus (GPa): 760
Hardness (GPa): 28 | Energy above hull (eV/atom): 0.47

Primitive Cell

1.000000

5.08411271637479	0.00000000000000	0.00000000000000
0.00000000000000	5.08411271637479	0.00000000000000
0.00000000000000	0.00000000000000	4.33559995005664

B N

8 8

DIRECT

0.6386865272328806	0.1386865272328806	0.5845619466548544
0.8613134727671194	0.3613134727671194	0.9154380533451457
0.3613134727671194	0.8613134727671194	0.5845619466548544
0.1386865272328806	0.6386865272328806	0.9154380533451457
0.3613134727671194	0.1386865272328806	0.0845619466548544
0.1386865272328806	0.3613134727671194	0.4154380533451457
0.6386865272328806	0.8613134727671194	0.0845619466548544
0.8613134727671194	0.6386865272328806	0.4154380533451457
0.1507833255050059	0.6507833255050059	0.5469444973468682
0.3492166744949941	0.8492166744949941	0.9530555026531319
0.8492166744949941	0.3492166744949941	0.5469444973468682
0.6507833255050059	0.1507833255050059	0.9530555026531319
0.8492166744949941	0.6507833255050059	0.0469444973468680
0.6507833255050059	0.8492166744949941	0.4530555026531318
0.1507833255050059	0.3492166744949941	0.0469444973468680
0.3492166744949941	0.1507833255050059	0.4530555026531318

Stiffness tensor (GPa):

517.624	321.994	67.676	-0.009	-0.011	0.010
321.994	517.659	67.709	0.002	-0.003	0.007
67.676	67.709	613.018	-0.010	-0.005	0.017
-0.009	0.002	-0.010	194.628	0.017	-0.054
-0.011	-0.003	-0.005	0.017	194.675	-0.001
0.010	0.007	0.017	-0.054	-0.001	351.938

BN-118

Density (g/cm^3): 2.93 | Space Group: 176
Bulk modulus (GPa): 301 | Shear modulus (GPa): 234
Young's modulus (GPa): 558 | Highest Young's modulus (GPa): 743
Hardness (GPa): 33 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

6.14645969187730	0.00000000000000	0.00000000000000
-3.07322984593865	5.32299023650282	0.00000000000000
0.00000000000000	0.00000000000000	2.58058389217250

B N

6 6

DIRECT

0.4062449006406847	0.3369897905301842	0.7500000000000000
0.5937550993593153	0.6630102094698158	0.2500000000000000
0.6630102094698158	0.0692551101105006	0.7500000000000000
0.3369897905301841	0.9307448898894994	0.2500000000000000
0.9307448898894994	0.5937550993593153	0.7500000000000000
0.0692551101105006	0.4062449006406847	0.2500000000000000
0.3137783404366691	0.4044947019624656	0.2500000000000000
0.6862216595633308	0.5955052980375344	0.7500000000000000
0.0907163615257964	0.6862216595633308	0.2500000000000000
0.9092836384742036	0.3137783404366692	0.7500000000000000
0.5955052980375344	0.9092836384742036	0.2500000000000000
0.4044947019624656	0.0907163615257964	0.7500000000000000

Stiffness tensor (GPa):

594.501	178.957	100.400	-0.019	-0.013	-0.005
178.957	594.266	100.050	0.001	0.013	0.053
100.400	100.050	768.612	0.007	0.015	0.049
-0.019	0.001	0.007	226.363	0.009	-0.010
-0.013	0.013	0.015	0.009	226.358	0.004
-0.005	0.053	0.049	-0.010	0.004	207.151

BN-119

Density (g/cm^3): 2.89 | Space Group: 57
Bulk modulus (GPa): 229 | Shear modulus (GPa): 183
Young's modulus (GPa): 433 | Highest Young's modulus (GPa): 570
Hardness (GPa): 29 | Energy above hull (eV/atom): 0.48

Primitive Cell

1.000000

4.54774765686394	0.00000000000000	0.00000000000000
0.00000000000000	4.73540888418976	0.00000000000000
0.00000000000000	0.00000000000000	7.94807924698035

B N

12 12

DIRECT

0.6351558696467864	0.4023156235604390	0.0962818446123270
0.3648441303532136	0.5976843764395610	0.9037181553876730
0.6351558696467864	0.0976843764395609	0.9037181553876730
0.3648441303532136	0.9023156235604390	0.0962818446123270
0.3648441303532136	0.5976843764395610	0.5962818446123270
0.6351558696467864	0.4023156235604390	0.4037181553876730
0.3648441303532136	0.9023156235604390	0.4037181553876730
0.6351558696467864	0.0976843764395609	0.5962818446123270
0.8648703539189233	0.4061080307806583	0.7500000000000000
0.1351296460810767	0.5938919692193416	0.2500000000000000
0.8648703539189233	0.0938919692193416	0.2500000000000000
0.1351296460810767	0.9061080307806584	0.7500000000000000
0.6615991297761985	0.4453786383281348	0.5978257608477295
0.3384008702238015	0.5546213616718652	0.4021742391522705
0.6615991297761985	0.0546213616718651	0.4021742391522705
0.3384008702238015	0.9453786383281348	0.5978257608477295
0.3384008702238015	0.5546213616718652	0.0978257608477295
0.6615991297761985	0.4453786383281348	0.9021742391522705
0.3384008702238015	0.9453786383281348	0.9021742391522705
0.6615991297761985	0.0546213616718651	0.0978257608477295
0.8459658589947461	0.4407075300135221	0.2500000000000000
0.1540341410052539	0.5592924699864779	0.7500000000000000
0.8459658589947461	0.0592924699864779	0.7500000000000000
0.1540341410052539	0.9407075300135221	0.2500000000000000

Stiffness tensor (GPa):

515.804	138.630	168.281	-0.022	-0.011	0.017
138.630	283.356	79.267	0.004	0.002	-0.008
168.281	79.267	629.241	-0.001	-0.005	0.018
-0.022	0.004	-0.001	179.608	0.001	0.012
-0.011	0.002	-0.005	0.001	204.589	-0.008
0.017	-0.008	0.018	0.012	-0.008	216.220

BN-120

Density (g/cm^3): 2.87 | Space Group: 36

Bulk modulus (GPa): 175 | Shear modulus (GPa): 175

Young's modulus (GPa): 394 | Highest Young's modulus (GPa): 662

Hardness (GPa): 38 | Energy above hull (eV/atom): 0.57

Primitive Cell

1.000000

1.30190624682679	-4.47666762123589	0.00000000000000
1.30190624682679	4.47666762123589	0.00000000000000
0.00000000000000	0.00000000000000	7.39121636006463

B N

6 6

DIRECT

0.0468526356863285	0.9531473643136715	0.9301235134544379
0.9531473643136715	0.0468526356863285	0.4301235134544379
0.2767388076445234	0.7232611923554766	0.4888993549985211
0.7232611923554766	0.2767388076445234	0.9888993549985211
0.6404107797147702	0.3595892202852298	0.6341674292733168
0.3595892202852298	0.6404107797147702	0.1341674292733168
0.8985028802694159	0.1014971197305841	0.0255887776483351
0.1014971197305841	0.8985028802694159	0.5255887776483351
0.8168738720211046	0.1831261279788954	0.5872680592014664
0.1831261279788954	0.8168738720211046	0.0872680592014663
0.4010676047105787	0.5989323952894213	0.3339534654982882
0.5989323952894213	0.4010676047105787	0.8339534654982882

Stiffness tensor (GPa):

681.474	73.556	45.330	-0.080	-0.045	0.008
73.556	371.114	27.236	-0.073	-0.049	0.009
45.330	27.236	322.806	-0.206	-0.047	-0.018
-0.080	-0.073	-0.206	132.571	0.021	0.033
-0.045	-0.049	-0.047	0.021	167.993	-0.016
0.008	0.009	-0.018	0.033	-0.016	193.677

BN-121

Density (g/cm^3): 2.86	Space Group: 21
Bulk modulus (GPa): 283	Shear modulus (GPa): 77
Young's modulus (GPa): 213	Highest Young's modulus (GPa): 848
Hardness (GPa): 3	Energy above hull (eV/atom): 0.45

Primitive Cell

1.000000

1.84799454361725	-1.84808268645734	0.00000000000000
1.84799454361725	1.84808268645734	0.00000000000000
0.00000000000000	0.00000000000000	14.74660718438485

B N

7 7

DIRECT

0.5000000000000000	0.5000000000000000	0.2991721009995455
0.5000000000000000	0.5000000000000000	0.7008278990004544
0.5000000000000000	0.0000000000000000	0.1533497444728247
0.0000000000000000	0.5000000000000000	0.8466502555271753
0.5000000000000000	0.0000000000000000	0.4441990188149383
0.0000000000000000	0.5000000000000000	0.5558009811850617
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.2027760560056744
0.5000000000000000	0.5000000000000000	0.7972239439943256
0.5000000000000000	0.0000000000000000	0.3486470263527621
0.0000000000000000	0.5000000000000000	0.6513529736472379
0.5000000000000000	0.0000000000000000	0.0578900812817396
0.0000000000000000	0.5000000000000000	0.9421099187182604
0.5000000000000000	0.5000000000000000	0.5000000000000000

Stiffness tensor (GPa):

583.556	4.989	143.813	0.568	0.174	0.074
4.989	583.578	143.554	-0.323	-0.384	-0.001
143.813	143.554	917.844	0.145	-0.176	-0.008
0.568	-0.323	0.145	10.789	0.080	-0.001
0.174	-0.384	-0.176	0.080	11.625	-0.000
0.074	-0.001	-0.008	-0.001	-0.000	36.157

BN-122

Density (g/cm^3): 2.85	Space Group: 223
Bulk modulus (GPa): 297	Shear modulus (GPa): 236
Young's modulus (GPa): 560	Highest Young's modulus (GPa): 690
Hardness (GPa): 34	Energy above hull (eV/atom): 0.30

Primitive Cell

1.000000

4.42759380158184	0.00000000000000	0.00000000000000
0.00000000000000	4.42759380158184	0.00000000000000
0.00000000000000	0.00000000000000	4.42759380158184

B N

6 6

DIRECT

0.5000000000000000	0.2500000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.7500000000000000
0.2500000000000000	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.2500000000000000
0.7500000000000000	0.0000000000000000	0.5000000000000000
0.0000000000000000	0.2500000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.7500000000000000
0.2500000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.2500000000000000
0.7500000000000000	0.5000000000000000	0.0000000000000000

Stiffness tensor (GPa):

710.328	90.506	90.507	0.004	0.007	-0.007
90.506	710.378	90.508	-0.004	-0.000	0.003
90.507	90.508	710.375	0.005	-0.006	-0.004
0.004	-0.004	0.005	196.644	-0.007	-0.002
0.007	-0.000	-0.006	-0.007	196.642	-0.005
-0.007	0.003	-0.004	-0.002	-0.005	196.647

BN-123

Density (g/cm^3): 2.85 | Space Group: 189
Bulk modulus (GPa): 284 | Shear modulus (GPa): 197
Young's modulus (GPa): 481 | Highest Young's modulus (GPa): 843
Hardness (GPa): 26 | Energy above hull (eV/atom): 0.23

Primitive Cell

```
   1.000000
     6.28103035938500      0.00000000000000      0.00000000000000
    -3.14051517969250      5.43953185316872      0.00000000000000
     0.00000000000000      0.00000000000000      2.54130644248295
   B     N
   6     6
DIRECT
     0.7332877107265677    0.7332877107265678    0.0000000000000000
     0.2667122892734323    0.0000000000000000    0.0000000000000000
    -0.0000000000000000    0.2667122892734322    0.0000000000000000
     0.6201648143422184    0.0000000000000000    0.5000000000000001
     0.0000000000000000    0.6201648143422185    0.5000000000000001
     0.3798351856577816    0.3798351856577816    0.5000000000000001
     0.2494058809023164    0.2494058809023164    0.0000000000000000
     0.7505941190976836    0.0000000000000000    0.0000000000000000
     0.0000000000000000    0.7505941190976836    0.0000000000000000
     0.3985038599022058    0.0000000000000000    0.5000000000000001
    -0.0000000000000000    0.3985038599022057    0.5000000000000001
     0.6014961400977943    0.6014961400977943    0.5000000000000001
```

Stiffness tensor (GPa):

478.337	193.596	97.093	-0.010	0.024	-0.060
193.596	477.731	96.658	0.009	-0.014	-0.029
97.093	96.658	870.973	-0.002	-0.001	0.004
-0.010	0.009	-0.002	208.812	0.006	-0.007
0.024	-0.014	-0.001	0.006	208.833	0.007
-0.060	-0.029	0.004	-0.007	0.007	141.485

BN-124

Density (g/cm^3): 2.84 | Space Group: 184
Bulk modulus (GPa): 292 | Shear modulus (GPa): 265
Young's modulus (GPa): 611 | Highest Young's modulus (GPa): 874
Hardness (GPa): 44 | Energy above hull (eV/atom): 0.32

Primitive Cell

1.000000

6.89869773772164	0.00000000000000	0.00000000000000
-3.44934886886082	5.97444749389717	0.00000000000000
0.00000000000000	0.00000000000000	4.22236918465809

B N

12 12

DIRECT

0.8818635354647930	0.3304927838483339	0.8173693061771408
0.6695072161516662	0.5513707516164591	0.8173693061771408
0.4486292483835408	0.1181364645352070	0.8173693061771408
0.1181364645352069	0.6695072161516662	0.8173693061771408
0.3304927838483339	0.4486292483835409	0.8173693061771408
0.5513707516164592	0.8818635354647930	0.8173693061771408
0.6695072161516662	0.1181364645352070	0.3173693061771408
0.4486292483835408	0.3304927838483339	0.3173693061771408
0.8818635354647930	0.5513707516164591	0.3173693061771408
0.3304927838483338	0.8818635354647930	0.3173693061771408
0.5513707516164592	0.6695072161516662	0.3173693061771408
0.1181364645352070	0.4486292483835409	0.3173693061771408
0.1250508502717073	0.6834640576157214	0.1826306973089153
0.3165359423842787	0.4415867926559861	0.1826306973089153
0.5584132073440140	0.8749491497282926	0.1826306973089153
0.8749491497282926	0.3165359423842787	0.1826306973089153
0.6834640576157214	0.5584132073440139	0.1826306973089153
0.4415867926559860	0.1250508502717074	0.1826306973089153
0.3165359423842786	0.8749491497282926	0.6826306973089153
0.5584132073440140	0.6834640576157214	0.6826306973089153
0.1250508502717074	0.4415867926559861	0.6826306973089153
0.6834640576157214	0.1250508502717074	0.6826306973089153
0.4415867926559860	0.3165359423842787	0.6826306973089153
0.8749491497282926	0.5584132073440139	0.6826306973089153

Stiffness tensor (GPa):

611.712	149.281	59.924	0.021	0.003	0.010
149.281	611.959	59.913	0.012	0.006	0.013
59.924	59.913	883.314	0.001	0.014	0.032
0.021	0.012	0.001	253.659	0.003	0.002
0.003	0.006	0.014	0.003	253.702	0.003
0.010	0.013	0.032	0.002	0.003	231.430

BN-125

Density (g/cm^3): 2.82 | Space Group: 8
Bulk modulus (GPa): 288 | Shear modulus (GPa): 197
Young's modulus (GPa): 482 | Highest Young's modulus (GPa): 548
Hardness (GPa): 25 | Energy above hull (eV/atom): 0.44

Primitive Cell

1.000000

6.45445566856659	-3.72648180361993	0.00000000000000
6.45445566856659	3.72648180361993	0.00000000000000
-4.30296966739147	0.00000000000000	6.08531978791668

B N

20 20

DIRECT

0.9999999191603175	0.3456083674683605	0.0000001019539698
0.9999999377246706	0.6543951537928288	0.0000000344398234
0.3456077354601864	0.0000000586941657	0.3456079085785970
0.6543944259791845	0.0000000156983054	0.6543945477586650
0.3456083674683605	0.9999999191603175	0.0000001019539698
0.6543951537928289	0.9999999377246704	0.0000000344398234
0.0000000156983054	0.6543944259791845	0.6543945477586650
0.0000000586941657	0.3456077354601864	0.3456079085785970
0.9999993329520762	0.9999993329520762	0.6543923184984854
0.9999994059113676	0.9999994059113675	0.3456053847345757
0.6543928035189341	0.3456059114019208	0.9999993425519343
0.3456059114019208	0.6543928035189341	0.9999993425519343
0.3864172077450383	0.8407484057200471	0.6135827268302755
0.6135823446364402	0.1592517854131533	0.3864172105621032
0.8407484057200471	0.3864172077450383	0.6135827268302755
0.1592517854131533	0.6135823446364402	0.3864172105621032
0.3864170569407578	0.3864170569407577	0.1592517301375338
0.6135827272010399	0.6135827272010398	0.8407483592970320
0.3864170943797899	0.3864170943797898	0.6135822959960366
0.6135828466318284	0.6135828466318283	0.3864171809941092
0.5000004887444194	0.8438034800584691	0.5000004600892849
0.5000006200818319	0.1561961506934464	0.5000004525715623
0.8438037412080333	0.5000006804203589	0.8438036968770271
0.1561961947186607	0.5000006969677628	0.1561960627984135
0.8438034800584691	0.5000004887444194	0.5000004600892849
0.1561961506934464	0.5000006200818319	0.5000004525715623
0.5000006969677628	0.1561961947186606	0.1561960627984135
0.5000006804203589	0.8438037412080333	0.8438036968770271
0.4999999499084570	0.4999999499084569	0.1561959928811352
0.5000000933400368	0.5000000933400368	0.8438040892904181
0.1561960322851184	0.8438039755073017	0.4999997802573819
0.8438039755073016	0.1561960322851185	0.4999997802573819
0.8760927889515946	0.3717216590099435	0.1239071300035005

0.1239085771113275	0.6282750786029441	0.8760917645923736
0.3717216590099435	0.8760927889515946	0.1239071300035005
0.6282750786029440	0.1239085771113276	0.8760917645923736
0.8760921444050429	0.8760921444050429	0.6282758964735116
0.1239074267368915	0.1239074267368914	0.3717223196196375
0.8760916101738572	0.8760916101738572	0.1239086950477109
0.1239070396970194	0.1239070396970193	0.8760929080459208

Stiffness tensor (GPa):

494.997	184.772	184.718	0.047	-0.013	0.009
184.772	495.050	184.766	0.045	-0.008	0.004
184.718	184.766	494.891	0.049	-0.007	0.018
0.047	0.045	0.049	231.375	-0.005	-0.004
-0.013	-0.008	-0.007	-0.005	231.368	0.003
0.009	0.004	0.018	-0.004	0.003	231.364

BN-126

Density (g/cm^3): 2.81 | Space Group: 217

Bulk modulus (GPa): 285 | Shear modulus (GPa): 173

Young's modulus (GPa): 431 | Highest Young's modulus (GPa): 537

Hardness (GPa): 20 | Energy above hull (eV/atom): 0.40

Primitive Cell

1.000000

-2.44681218135683	2.44681218135683	2.44681218135683
2.44681218135683	-2.44681218135683	2.44681218135683
2.44681218135683	2.44681218135683	-2.44681218135683

B N

4 4

DIRECT

0.6855984461452471	0.0000000000000000	0.0000000000000000
0.3144015538547529	0.3144015538547529	0.3144015538547529
0.0000000000000000	0.0000000000000000	0.6855984461452471
0.0000000000000000	0.6855984461452471	0.0000000000000000
0.3383080142983563	0.0000000000000000	0.0000000000000000
0.6616919857016437	0.6616919857016437	0.6616919857016437
0.0000000000000000	0.0000000000000000	0.3383080142983563
0.0000000000000000	0.3383080142983563	0.0000000000000000

Stiffness tensor (GPa):

438.353	208.457	208.438	0.042	-0.027	-0.001
208.457	438.300	208.458	-0.029	0.035	-0.003
208.438	208.458	438.322	-0.033	-0.024	0.074
0.042	-0.029	-0.033	226.554	-0.011	-0.013
-0.027	0.035	-0.024	-0.011	226.559	-0.012
-0.001	-0.003	0.074	-0.013	-0.012	226.579

BN-127

Density (g/cm^3): 2.76 | Space Group: 18

Bulk modulus (GPa): 186 | Shear modulus (GPa): 151

Young's modulus (GPa): 356 | Highest Young's modulus (GPa): 701

Hardness (GPa): 26 | Energy above hull (eV/atom): 0.37

Primitive Cell

1.000000

4.50696513918197	0.00000000000000	0.00000000000000
0.00000000000000	5.24832382927130	0.00000000000000
0.00000000000000	0.00000000000000	7.57249492278686

B N

12 12

DIRECT

0.3459193056238157	0.2483963503065747	0.5826689138916432
0.6540806943761843	0.7516036496934253	0.5826689138916432
0.1540806943761843	0.7483963503065747	0.4173310861083568
0.8459193056238157	0.2516036496934253	0.4173310861083568
0.6625761675168932	0.3344979139224835	0.0681717739617258
0.3374238324831068	0.6655020860775165	0.0681717739617258
0.8374238324831068	0.8344979139224835	0.9318282260382742
0.1625761675168933	0.1655020860775165	0.9318282260382742
0.8535243748839443	0.2347464036168390	0.7398225799374578
0.1464756251160557	0.7652535963831610	0.7398225799374578
0.6464756251160557	0.7347464036168390	0.2601774200625422
0.3535243748839443	0.2652535963831610	0.2601774200625422
0.1718694868758415	0.2521217304019421	0.4163800897370598
0.8281305131241585	0.7478782695980579	0.4163800897370598
0.3281305131241585	0.7521217304019421	0.5836199102629402
0.6718694868758415	0.2478782695980579	0.5836199102629402
0.8065185152630026	0.1611945005515674	0.9329503479949521
0.1934814847369974	0.8388054994484326	0.9329503479949521
0.6934814847369974	0.6611945005515674	0.0670496520050479
0.3065185152630026	0.3388054994484326	0.0670496520050479
0.6715260647458563	0.2520936803500162	0.2596894293021168
0.3284739352541437	0.7479063196499838	0.2596894293021168
0.8284739352541437	0.7520936803500162	0.7403105706978832
0.1715260647458563	0.2479063196499838	0.7403105706978832

Stiffness tensor (GPa):

610.208	32.972	190.968	0.074	0.073	0.016
32.972	161.575	74.603	0.029	0.151	0.010
190.968	74.603	763.185	-0.030	0.054	0.023
0.074	0.029	-0.030	85.797	-0.025	0.008
0.073	0.151	0.054	-0.025	290.131	-0.011
0.016	0.010	0.023	0.008	-0.011	95.879

BN-128

Density (g/cm^3): 2.75 | Space Group: 36

Bulk modulus (GPa): 197 | Shear modulus (GPa): 181

Young's modulus (GPa): 416 | Highest Young's modulus (GPa): 481

Hardness (GPa): 35 | Energy above hull (eV/atom): 0.61

Primitive Cell

1.000000

4.04300184765531	-2.49715396896111	0.00000000000000
4.04300184765531	2.49715396896111	0.00000000000000
0.00000000000000	0.00000000000000	4.45664764367588

B N

6 6

DIRECT

0.1069048769523626	0.8930951230476374	0.8971941145528748
0.8930951230476374	0.1069048769523626	0.3971941145528748
0.6607101493863594	0.9493652730092930	0.0853946923272718
0.3392898506136405	0.0506347269907071	0.5853946923272718
0.9493652730092930	0.6607101493863594	0.5853946923272718
0.0506347269907071	0.3392898506136405	0.0853946923272718
0.8340015221495628	0.1659984778504372	0.0506626859440348
0.1659984778504371	0.8340015221495629	0.5506626859440348
0.3449039718636744	0.0512904240675559	0.9406769045820705
0.6550960281363254	0.9487095759324442	0.4406769045820704
0.0512904240675559	0.3449039718636746	0.4406769045820704
0.9487095759324440	0.6550960281363256	0.9406769045820705

Stiffness tensor (GPa):

474.361	162.285	96.324	-0.058	0.004	-0.027
162.285	326.423	30.609	-0.079	-0.015	-0.050
96.324	30.609	445.758	-0.042	-0.004	-0.022
-0.058	-0.079	-0.042	183.804	0.003	0.001
0.004	-0.015	-0.004	0.003	223.168	-0.026
-0.027	-0.050	-0.022	0.001	-0.026	209.047

BN-129

Density (g/cm^3): 2.74 | Space Group: 70
Bulk modulus (GPa): 244 | Shear modulus (GPa): 155
Young's modulus (GPa): 383 | Highest Young's modulus (GPa): 602
Hardness (GPa): 19 | Energy above hull (eV/atom): 0.46

Primitive Cell

1.000000

0.00000000000000	3.41317284812047	3.51054403923444
2.50695189594577	0.00000000000000	3.51054403923444
2.50695189594577	3.41317284812047	0.00000000000000

B N

4 4

DIRECT

0.5999311935290237	0.5999311935290237	0.9000688064709763
0.6500688064709763	0.6500688064709763	0.3499311935290237
0.9000688064709763	0.9000688064709763	0.5999311935290237
0.3499311935290237	0.3499311935290237	0.6500688064709763
0.6782533673939415	0.3217466326060585	0.6782533673939415
0.5717466326060585	0.9282533673939415	0.5717466326060585
0.3217466326060585	0.6782533673939415	0.3217466326060585
0.9282533673939415	0.5717466326060585	0.9282533673939415

Stiffness tensor (GPa):

560.298	192.210	237.212	-0.068	-0.002	0.019
192.210	346.130	81.747	-0.001	0.001	-0.012
237.212	81.747	413.972	-0.005	-0.003	-0.001
-0.068	-0.001	-0.005	82.666	0.005	-0.028
-0.002	0.001	-0.003	0.005	293.359	-0.009
0.019	-0.012	-0.001	-0.028	-0.009	212.693

BN-130

Density (g/cm^3): 2.74 | Space Group: 126
Bulk modulus (GPa): 230 | Shear modulus (GPa): 158
Young's modulus (GPa): 385 | Highest Young's modulus (GPa): 565
Hardness (GPa): 22 | Energy above hull (eV/atom): 0.49

Primitive Cell

1.000000

7.10152210863265	0.00000000000000	0.00000000000000
0.00000000000000	7.10152210863265	0.00000000000000
0.00000000000000	0.00000000000000	4.77054535763700

B N

16 16

DIRECT

0.1129149128515885	0.7360243852902528	0.3484866274607021
0.8870850871484115	0.2639756147097472	0.3484866274607021
0.2360243852902526	0.3870850871484114	0.1515133725392979
0.7639756147097473	0.6129149128515885	0.1515133725392979
0.8870850871484115	0.7360243852902528	0.6515133725392979
0.1129149128515885	0.2639756147097472	0.6515133725392979
0.7639756147097473	0.3870850871484114	0.8484866274607021
0.2360243852902526	0.6129149128515885	0.8484866274607021
0.3870850871484114	0.7639756147097473	0.1515133725392979
0.6129149128515885	0.2360243852902526	0.1515133725392979
0.2639756147097472	0.1129149128515885	0.3484866274607021
0.7360243852902528	0.8870850871484115	0.3484866274607021
0.6129149128515885	0.7639756147097473	0.8484866274607021
0.3870850871484114	0.2360243852902526	0.8484866274607021
0.7360243852902528	0.1129149128515885	0.6515133725392979
0.2639756147097472	0.8870850871484115	0.6515133725392979
0.9014881989697610	0.2610554344757579	0.6918886403200526
0.0985118010302390	0.7389445655242421	0.6918886403200526
0.7610554344757580	0.5985118010302390	0.8081113596799474
0.2389445655242420	0.4014881989697609	0.8081113596799474
0.0985118010302390	0.2610554344757579	0.3081113596799474
0.9014881989697610	0.7389445655242421	0.3081113596799474
0.2389445655242420	0.5985118010302390	0.1918886403200526
0.7610554344757580	0.4014881989697609	0.1918886403200526
0.5985118010302390	0.2389445655242420	0.8081113596799474
0.4014881989697609	0.7610554344757580	0.8081113596799474
0.7389445655242421	0.9014881989697610	0.6918886403200526
0.2610554344757579	0.0985118010302390	0.6918886403200526
0.4014881989697609	0.2389445655242420	0.1918886403200526
0.5985118010302390	0.7610554344757580	0.1918886403200526
0.2610554344757579	0.9014881989697610	0.3081113596799474
0.7389445655242421	0.0985118010302390	0.3081113596799474

Stiffness tensor (GPa):

619.778	91.783	121.588	-0.003	-0.016	-0.002
91.783	619.776	121.637	-0.022	-0.003	0.010
121.588	121.637	282.166	-0.028	-0.011	0.017
-0.003	-0.022	-0.028	190.751	0.008	-0.000
-0.016	-0.003	-0.011	0.008	190.735	-0.004
-0.002	0.010	0.017	-0.000	-0.004	83.102

BN-131

Density (g/cm^3): 2.74 | Space Group: 185
Bulk modulus (GPa): 279 | Shear modulus (GPa): 211
Young's modulus (GPa): 506 | Highest Young's modulus (GPa): 839
Hardness (GPa): 30 | Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

6.97685790958048	0.00000000000000	0.00000000000000
-3.48842895479024	6.04213618829109	0.00000000000000
0.00000000000000	0.00000000000000	4.28429191581079

B N

12 12

DIRECT

-0.0000000000000000	0.2163347315808092	0.9360777341066779
0.7836652684191908	0.7836652684191908	0.9360777341066779
0.2163347315808092	0.0000000000000000	0.9360777341066779
0.0000000000000000	0.7836652684191908	0.4360777341066779
0.2163347315808092	0.2163347315808092	0.4360777341066779
0.7836652684191908	0.0000000000000000	0.4360777341066779
-0.0000000000000000	0.4115370177217946	0.4154670895698966
0.5884629822782054	0.5884629822782055	0.4154670895698966
0.4115370177217946	0.0000000000000000	0.4154670895698966
0.0000000000000000	0.5884629822782055	0.9154670895698966
0.4115370177217946	0.4115370177217946	0.9154670895698966
0.5884629822782054	0.0000000000000000	0.9154670895698966
0.0000000000000000	0.7860281546007951	0.0649001801329247
0.2139718453992049	0.2139718453992049	0.0649001801329247
0.7860281546007951	0.0000000000000000	0.0649001801329247
-0.0000000000000000	0.2139718453992049	0.5649001801329248
0.7860281546007951	0.7860281546007951	0.5649001801329248
0.2139718453992049	0.0000000000000000	0.5649001801329248
0.0000000000000000	0.5861023094729474	0.5835549993256618
0.4138976905270526	0.4138976905270526	0.5835549993256618
0.5861023094729474	0.0000000000000000	0.5835549993256618
-0.0000000000000000	0.4138976905270526	0.0835549993256617
0.5861023094729474	0.5861023094729474	0.0835549993256617
0.4138976905270526	0.0000000000000000	0.0835549993256617

Stiffness tensor (GPa):

492.590	180.753	84.014	-0.005	0.008	0.018
180.753	493.542	84.424	-0.007	0.006	0.011
84.014	84.424	859.743	-0.040	-0.007	0.012
-0.005	-0.007	-0.040	223.829	0.004	-0.001
0.008	0.006	-0.007	0.004	223.837	-0.028
0.018	0.011	0.012	-0.001	-0.028	155.519

BN-132

Density (g/cm^3): 2.70 | Space Group: 129
Bulk modulus (GPa): 218 | Shear modulus (GPa): 146
Young's modulus (GPa): 359 | Highest Young's modulus (GPa): 692
Hardness (GPa): 20 | Energy above hull (eV/atom): 0.39

Primitive Cell

1.000000

7.53832697411342	0.00000000000000	0.00000000000000
0.00000000000000	7.53832697411342	0.00000000000000
0.00000000000000	0.00000000000000	4.29856174400851

B N

16 16

DIRECT

0.6741213299257547	0.1741213299257547	0.1777903981014819
0.8258786700742453	0.3258786700742454	0.8222096018985181
0.3258786700742454	0.8258786700742453	0.1777903981014819
0.1741213299257547	0.6741213299257547	0.8222096018985181
0.3258786700742454	0.1741213299257547	0.1777903981014819
0.1741213299257547	0.3258786700742454	0.8222096018985181
0.6741213299257547	0.8258786700742453	0.1777903981014819
0.8258786700742453	0.6741213299257547	0.8222096018985181
0.0000000000000000	0.7180488580111448	0.3536352955898824
0.4999999999999999	0.7819511419888552	0.6463647044101175
0.0000000000000000	0.2819511419888552	0.3536352955898824
0.4999999999999999	0.2180488580111449	0.6463647044101175
0.7819511419888552	0.4999999999999999	0.3536352955898824
0.7180488580111448	0.0000000000000000	0.6463647044101175
0.2180488580111449	0.4999999999999999	0.3536352955898824
0.2819511419888552	0.0000000000000000	0.6463647044101175
0.1709748329676104	0.6709748329676104	0.1877796968545088
0.3290251670323897	0.8290251670323896	0.8122203031454913
0.8290251670323896	0.3290251670323897	0.1877796968545088
0.6709748329676104	0.1709748329676104	0.8122203031454913
0.8290251670323896	0.6709748329676104	0.1877796968545088
0.6709748329676104	0.8290251670323896	0.8122203031454913
0.1709748329676104	0.3290251670323897	0.1877796968545088
0.3290251670323897	0.1709748329676104	0.8122203031454913
0.4999999999999999	0.2375412602586571	0.3225713789918870
0.0000000000000000	0.2624587397413430	0.6774286210081131
0.4999999999999999	0.7624587397413429	0.3225713789918870
0.0000000000000000	0.7375412602586571	0.6774286210081131
0.2624587397413430	0.0000000000000000	0.3225713789918870
0.2375412602586571	0.4999999999999999	0.6774286210081131
0.7375412602586571	0.0000000000000000	0.3225713789918870
0.7624587397413429	0.4999999999999999	0.6774286210081131

Stiffness tensor (GPa):

363.322	136.402	75.676	-0.010	-0.020	0.030
136.402	363.455	75.690	0.012	-0.005	0.020
75.676	75.690	715.275	-0.042	-0.000	0.023
-0.010	0.012	-0.042	168.581	0.008	-0.001
-0.020	-0.005	-0.000	0.008	168.577	-0.019
0.030	0.020	0.023	-0.001	-0.019	77.058

BN-133

Density (g/cm^3): 2.69 | Space Group: 156

Bulk modulus (GPa): 201 | Shear modulus (GPa): 117

Young's modulus (GPa): 294 | Highest Young's modulus (GPa): 493

Hardness (GPa): 14 | Energy above hull (eV/atom): 0.27

Primitive Cell

1.000000

7.14513892260647	0.00000000000000	0.00000000000000
-3.57256946130324	6.18787182054618	0.00000000000000
0.00000000000000	0.00000000000000	3.11585485539925

B N

9 9

DIRECT

0.8840852804437549	0.1159147195562451	0.0491882983566660
0.2174182129449641	0.4348364258899281	0.7158539874774265
0.5651635741100720	0.7825817870550360	0.7158539874774265
0.5507517062348681	0.4492482937651321	0.3825199586628052
0.8840852804437549	0.7681705608875098	0.0491882983566660
0.2318294391124902	0.1159147195562451	0.0491882983566660
0.2174182129449640	0.7825817870550360	0.7158539874774265
0.5507517062348680	0.1015034124697361	0.3825199586628052
0.8984965875302640	0.4492482937651321	0.3825199586628052
0.7843575563882739	0.2156424436117261	0.2841453234723628
0.1176914667236542	0.2353829334473084	0.9508142245038834
0.7646170665526917	0.8823085332763458	0.9508142245038834
0.4510246175605926	0.5489753824394072	0.6174782093641149
0.7843575563882739	0.5687151127765476	0.2841453234723628
0.4312848872234523	0.2156424436117262	0.2841453234723628
0.1176914667236541	0.8823085332763458	0.9508142245038834
0.4510246175605926	0.9020492351211853	0.6174782093641149
0.0979507648788147	0.5489753824394072	0.6174782093641149

Stiffness tensor (GPa):

658.873	300.523	113.737	-16.733	0.022	0.025
300.523	658.049	113.022	16.580	-0.029	0.050
113.737	113.022	124.510	-0.065	-0.010	0.064
-16.733	16.580	-0.065	95.843	-0.007	0.015
0.022	-0.029	-0.010	-0.007	95.903	-16.626
0.025	0.050	0.064	0.015	-16.626	178.644

BN-134

Density (g/cm^3): 2.68 | Space Group: 165

Bulk modulus (GPa): 260 | Shear modulus (GPa): 203

Young's modulus (GPa): 483 | Highest Young's modulus (GPa): 554

Hardness (GPa): 31 | Energy above hull (eV/atom): 0.46

Primitive Cell

1.000000

6.97477376943313	0.00000000000000	0.00000000000000
-3.48738688471657	6.04033126997844	0.00000000000000
0.00000000000000	0.00000000000000	4.38533236167129

B N

12 12

DIRECT

0.1281639712930887	0.4619539095373515	0.9188369441731070
0.8718360287069113	0.5380460904626485	0.0811630558268930
0.5380460904626485	0.6662100617557372	0.9188369441731070
0.4619539095373515	0.3337899382442629	0.0811630558268930
0.3337899382442629	0.8718360287069113	0.9188369441731070
0.6662100617557372	0.1281639712930887	0.0811630558268930
0.4619539095373515	0.1281639712930887	0.5811630558268930
0.5380460904626485	0.8718360287069113	0.4188369441731070
0.6662100617557372	0.5380460904626485	0.5811630558268930
0.3337899382442629	0.4619539095373515	0.4188369441731070
0.8718360287069113	0.3337899382442629	0.5811630558268930
0.1281639712930887	0.6662100617557372	0.4188369441731070
0.8671610377592047	0.5469029400034247	0.4394293651702199
0.1328389622407953	0.4530970599965753	0.5605706348297801
0.4530970599965753	0.3202580977557801	0.4394293651702199
0.5469029400034247	0.6797419022442199	0.5605706348297801
0.6797419022442199	0.1328389622407953	0.4394293651702199
0.3202580977557801	0.8671610377592047	0.5605706348297801
0.5469029400034247	0.8671610377592047	0.0605706348297801
0.4530970599965753	0.1328389622407953	0.9394293651702199
0.3202580977557801	0.4530970599965753	0.0605706348297801
0.6797419022442199	0.5469029400034247	0.9394293651702199
0.1328389622407953	0.6797419022442199	0.0605706348297801
0.8671610377592047	0.3202580977557801	0.9394293651702199

Stiffness tensor (GPa):

518.810	151.413	102.875	-4.284	0.010	-0.055
151.413	518.870	102.871	4.011	-0.026	0.015
102.875	102.871	585.901	-0.038	0.004	-0.010
-4.284	4.011	-0.038	207.025	0.003	0.003
0.010	-0.026	0.004	0.003	207.053	-3.955
-0.055	0.015	-0.010	0.003	-3.955	184.007

BN-135

Density (g/cm^3): 2.67 | Space Group: 216

Bulk modulus (GPa): 265 | Shear modulus (GPa): 209

Young's modulus (GPa): 497 | Highest Young's modulus (GPa): 570

Hardness (GPa): 32 | Energy above hull (eV/atom): 0.46

Primitive Cell

1.000000

0.00000000000000	3.37901026629815	3.37901026629815
3.37901026629815	0.00000000000000	3.37901026629815
3.37901026629815	3.37901026629815	0.00000000000000

B N

5 5

DIRECT

0.6619361444106086	0.1126879518631304	0.1126879518631306
0.1126879518631307	0.6619361444106087	0.1126879518631304
0.1126879518631304	0.1126879518631304	0.6619361444106087
0.1126879518631304	0.1126879518631304	0.1126879518631307
0.7500000000000000	0.7500000000000000	0.7500000000000000
0.3619139872158796	0.8793620042613735	0.8793620042613735
0.8793620042613735	0.3619139872158796	0.8793620042613735
0.8793620042613735	0.8793620042613735	0.3619139872158796
0.8793620042613735	0.8793620042613735	0.8793620042613735
0.2500000000000000	0.2500000000000000	0.2500000000000000

Stiffness tensor (GPa):

479.531	157.206	157.231	0.063	-0.027	-0.043
157.206	479.432	157.233	-0.130	-0.005	0.046
157.231	157.233	479.418	0.024	-0.115	-0.010
0.063	-0.130	0.024	249.431	-0.028	-0.013
-0.027	-0.005	-0.115	-0.028	249.494	-0.056
-0.043	0.046	-0.010	-0.013	-0.056	249.487

BN-136

Density (g/cm^3): 2.62 | Space Group: 57

Bulk modulus (GPa): 237 | Shear modulus (GPa): 145

Young's modulus (GPa): 362 | Highest Young's modulus (GPa): 697

Hardness (GPa): 18 | Energy above hull (eV/atom): 0.29

Primitive Cell

1.000000

6.25425765314473	0.00000000000000	0.00000000000000
0.00000000000000	4.31958211165327	0.00000000000000
0.00000000000000	0.00000000000000	11.64191832004172

B N

20 20

DIRECT

0.7350783672310939	0.1000126825627163	0.6487274253192232
0.2649216327689061	0.8999873174372837	0.3512725746807767
0.7350783672310939	0.3999873174372837	0.3512725746807767
0.2649216327689061	0.6000126825627163	0.6487274253192232
0.2649216327689061	0.8999873174372837	0.1487274253192232
0.7350783672310939	0.1000126825627163	0.8512725746807768
0.2649216327689061	0.6000126825627163	0.8512725746807768
0.7350783672310939	0.3999873174372837	0.1487274253192232
0.1178779344446361	0.0782232706170657	0.5679496930742576
0.8821220655553639	0.9217767293829343	0.4320503069257425
0.1178779344446361	0.4217767293829343	0.4320503069257425
0.8821220655553639	0.5782232706170657	0.5679496930742576
0.8821220655553639	0.9217767293829343	0.0679496930742576
0.1178779344446361	0.0782232706170657	0.9320503069257425
0.8821220655553639	0.5782232706170657	0.9320503069257425
0.1178779344446361	0.4217767293829343	0.0679496930742576
0.3760317450444023	0.4287289968325121	0.2500000000000000
0.6239682549555977	0.5712710031674879	0.7500000000000000
0.3760317450444023	0.0712710031674879	0.7500000000000000
0.6239682549555977	0.9287289968325121	0.2500000000000000
0.7227596557081321	0.0758518530136610	0.1419551155200945
0.2772403442918679	0.9241481469863390	0.8580448844799056
0.7227596557081321	0.4241481469863390	0.8580448844799056
0.2772403442918679	0.5758518530136610	0.1419551155200945
0.2772403442918679	0.9241481469863390	0.6419551155200944
0.7227596557081321	0.0758518530136610	0.3580448844799055
0.2772403442918679	0.5758518530136610	0.3580448844799055
0.7227596557081321	0.4241481469863390	0.6419551155200944
0.1190852554755990	0.0671523882933346	0.0735583078098841
0.8809147445244010	0.9328476117066654	0.9264416921901160
0.1190852554755990	0.4328476117066654	0.9264416921901160
0.8809147445244010	0.5671523882933346	0.0735583078098841
0.8809147445244010	0.9328476117066654	0.5735583078098840

0.1190852554755990	0.0671523882933346	0.4264416921901159
0.8809147445244010	0.5671523882933346	0.4264416921901159
0.1190852554755990	0.4328476117066654	0.5735583078098840
0.3723803143587727	0.4408971799796766	0.7500000000000000
0.6276196856412273	0.5591028200203234	0.2500000000000000
0.3723803143587727	0.0591028200203234	0.2500000000000000
0.6276196856412273	0.9408971799796766	0.7500000000000000

Stiffness tensor (GPa):

310.024	84.499	234.974	0.002	0.019	0.013
84.499	724.238	88.709	0.003	-0.017	0.032
234.974	88.709	323.802	0.013	-0.042	0.042
0.002	0.003	0.013	220.499	0.031	-0.006
0.019	-0.017	-0.042	0.031	173.610	0.029
0.013	0.032	0.042	-0.006	0.029	174.951

BN-137

Density (g/cm^3): 2.61 | Space Group: 72
Bulk modulus (GPa): 230 | Shear modulus (GPa): 134
Young's modulus (GPa): 337 | Highest Young's modulus (GPa): 677
Hardness (GPa): 16 | Energy above hull (eV/atom): 0.29

Primitive Cell

1.000000

-2.17877413681071	6.14201328701507	5.89911132214635
2.17877413681071	-6.14201328701507	5.89911132214635
2.17877413681071	6.14201328701507	-5.89911132214635

B N

20 20

DIRECT

0.9834215427281414	0.7507540606786309	0.5323583864867050
0.0165784572718586	0.2492459393213690	0.4676416135132950
0.2183956741919260	0.4510631562414364	0.4676416135132950
0.7816043258080740	0.5489368437585636	0.5323583864867050
0.2816043258080740	0.7492459393213691	0.2326674820495104
0.7183956741919260	0.2507540606786309	0.7673325179504895
0.5165784572718586	0.0489368437585635	0.7673325179504895
0.4834215427281414	0.9510631562414364	0.2326674820495104
0.9930817580831740	0.3547462772530999	0.9818535007608542
0.0069182419168259	0.6452537227469000	0.0181464992391458
0.3728927764922457	0.0112282573223198	0.0181464992391458
0.6271072235077542	0.9887717426776801	0.9818535007608542
0.1271072235077542	0.1452537227469000	0.6383354808300741
0.8728927764922457	0.8547462772530999	0.3616645191699259
0.5069182419168259	0.4887717426776801	0.3616645191699259
0.4930817580831740	0.5112282573223198	0.6383354808300741
0.9325302914671649	0.1744192652414754	0.1069495567086403
0.0674697085328351	0.8255807347585247	0.8930504432913597
0.4325302914671649	0.3255807347585247	0.7581110262256896
0.5674697085328351	0.6744192652414753	0.2418889737743104
0.4951313272820509	0.2793210243471646	0.5610289490828650
0.5048686727179490	0.7206789756528353	0.4389710509171350
0.7182920752642996	0.9341023781991858	0.4389710509171350
0.2817079247357004	0.0658976218008141	0.5610289490828650
0.7817079247357004	0.2206789756528353	0.2158103029348863
0.2182920752642996	0.7793210243471647	0.7841896970651137
0.0048686727179491	0.5658976218008140	0.7841896970651137
0.9951313272820509	0.4341023781991858	0.2158103029348863
0.4901471842359820	0.8615141205943294	0.9944940963523337
0.5098528157640181	0.1384858794056706	0.0055059036476663
0.8670200242419958	0.4956530878836484	0.0055059036476663
0.1329799757580043	0.5043469121163517	0.9944940963523337
0.6329799757580044	0.6384858794056707	0.6286330636416526

0.3670200242419958	0.3615141205943294	0.3713669363583474
0.0098528157640180	0.0043469121163517	0.3713669363583474
0.9901471842359820	0.9956530878836484	0.6286330636416526
0.4292716030477681	0.6845012860111739	0.1137728890589420
0.5707283969522319	0.3154987139888261	0.8862271109410580
0.9292716030477681	0.8154987139888261	0.7447703170365942
0.0707283969522319	0.1845012860111739	0.2552296829634058

Stiffness tensor (GPa):

716.752	95.551	107.656	-0.011	0.003	0.030
95.551	256.309	220.927	-0.043	-0.003	0.067
107.656	220.927	349.572	0.028	0.006	0.095
-0.011	-0.043	0.028	141.216	-0.065	-0.004
0.003	-0.003	0.006	-0.065	229.651	-0.010
0.030	0.067	0.095	-0.004	-0.010	151.549

BN-138

Density (g/cm^3): 2.59 | Space Group: 46

Bulk modulus (GPa): 194 | Shear modulus (GPa): 128

Young's modulus (GPa): 314 | Highest Young's modulus (GPa): 727

Hardness (GPa): 18 | Energy above hull (eV/atom): 0.21

Primitive Cell

1.000000

-2.46644726583001	1.59989320561320	4.02620949415112
2.46644726583001	-1.59989320561320	4.02620949415112
2.46644726583001	1.59989320561320	-4.02620949415112

B N

4 4

DIRECT

0.4120023221118367	0.9120023221118367	0.5000000000000000
0.4120023221118367	0.4120023221118367	0.0000000000000000
0.5486340710667426	0.4233490935283516	0.6252849775383909
0.7980641159899607	0.9233490935283517	0.3747150224616091
0.5900426045250633	0.0900426045250633	0.5000000000000000
0.5900426045250633	0.5900426045250633	0.0000000000000000
0.4508772087945867	0.5746059777977153	0.3762712309968714
0.1983347468008438	0.0746059777977153	0.6237287690031286

Stiffness tensor (GPa):

809.437	62.434	238.027	-0.022	0.043	0.018
62.434	122.596	127.893	-0.077	0.054	0.037
238.027	127.893	648.036	-0.076	0.027	0.038
-0.022	-0.077	-0.076	69.997	0.008	0.002
0.043	0.054	0.027	0.008	287.384	0.001
0.018	0.037	0.038	0.002	0.001	70.807

BN-139

Density (g/cm^3): 2.59 | Space Group: 111

Bulk modulus (GPa): 179 | Shear modulus (GPa): 108

Young's modulus (GPa): 270 | Highest Young's modulus (GPa): 401

Hardness (GPa): 14 | Energy above hull (eV/atom): 0.75

Primitive Cell

1.000000

4.89395911931373	0.00000000000000	0.00000000000000
0.00000000000000	4.89395911931373	0.00000000000000
0.00000000000000	0.00000000000000	7.96443783418904

B N

12 12

DIRECT

0.6631552205845150	0.6631552205845150	0.2148318879617088
0.3368447794154850	0.3368447794154850	0.2148318879617088
0.6631552205845150	0.3368447794154850	0.7851681120382912
0.3368447794154850	0.6631552205845150	0.7851681120382912
0.3531675868416990	0.3531675868416990	0.5941829071476659
0.6468324131583010	0.6468324131583010	0.5941829071476659
0.3531675868416990	0.6468324131583010	0.4058170928523341
0.6468324131583010	0.3531675868416990	0.4058170928523341
0.1565762787072412	0.1565762787072412	0.9021917610928444
0.8434237212927588	0.8434237212927588	0.9021917610928444
0.1565762787072412	0.8434237212927588	0.0978082389071556
0.8434237212927588	0.1565762787072412	0.0978082389071556
0.3274793897116656	0.3274793897116656	0.7907157039308301
0.6725206102883344	0.6725206102883344	0.7907157039308301
0.3274793897116656	0.6725206102883344	0.2092842960691698
0.6725206102883344	0.3274793897116656	0.2092842960691698
0.6855367417663760	0.6855367417663760	0.4072225778975436
0.3144632582336240	0.3144632582336240	0.4072225778975436
0.6855367417663760	0.3144632582336240	0.5927774221024564
0.3144632582336240	0.6855367417663760	0.5927774221024564
0.8297962369111824	0.8297962369111824	0.1016562814717158
0.1702037630888176	0.1702037630888176	0.1016562814717158
0.8297962369111824	0.1702037630888176	0.8983437185282842
0.1702037630888176	0.8297962369111824	0.8983437185282842

Stiffness tensor (GPa):

231.198	99.151	141.702	-0.022	0.217	0.015
99.151	231.250	141.705	-0.007	-0.078	-0.003
141.702	141.705	523.020	-0.015	-0.009	-0.076
-0.022	-0.007	-0.015	113.224	-0.364	-0.077
0.217	-0.078	-0.009	-0.364	113.585	0.014
0.015	-0.003	-0.076	-0.077	0.014	141.068

BN-140

Density (g/cm^3): 2.58 | Space Group: 136
Bulk modulus (GPa): 151 | Shear modulus (GPa): 119
Young's modulus (GPa): 282 | Highest Young's modulus (GPa): 578
Hardness (GPa): 22 | Energy above hull (eV/atom): 0.63

Primitive Cell

1.000000

8.59487024240954	0.00000000000000	0.00000000000000
0.00000000000000	8.59487024240954	0.00000000000000
0.00000000000000	0.00000000000000	2.59999174924534

B N

12 12

DIRECT

0.2371419519597481	0.7628580480402518	0.0000000000000000
0.7628580480402518	0.2371419519597482	0.0000000000000000
0.7371419519597482	0.7371419519597482	0.5000000000000000
0.2628580480402518	0.2628580480402519	0.5000000000000000
0.1715723949189555	0.4260454907990567	0.0000000000000000
0.8284276050810445	0.5739545092009433	0.0000000000000000
0.5739545092009433	0.8284276050810445	0.0000000000000000
0.4260454907990567	0.1715723949189555	0.0000000000000000
0.9260454907990567	0.3284276050810445	0.5000000000000000
0.0739545092009433	0.6715723949189555	0.5000000000000000
0.3284276050810445	0.9260454907990567	0.5000000000000000
0.6715723949189555	0.0739545092009433	0.5000000000000000
0.3333454026220002	0.3333454026220002	0.0000000000000000
0.6666545973779998	0.6666545973779998	0.0000000000000000
0.8333454026220002	0.1666545973779998	0.5000000000000000
0.1666545973779998	0.8333454026220002	0.5000000000000000
0.3977944145472542	0.8478630149264016	0.0000000000000000
0.6022055854527458	0.1521369850735984	0.0000000000000000
0.8478630149264016	0.3977944145472542	0.0000000000000000
0.1521369850735984	0.6022055854527458	0.0000000000000000
0.6521369850735984	0.8977944145472542	0.5000000000000000
0.3478630149264017	0.1022055854527458	0.5000000000000000
0.1022055854527458	0.3478630149264017	0.5000000000000000
0.8977944145472542	0.6521369850735984	0.5000000000000000

Stiffness tensor (GPa):

197.219	108.931	60.513	-0.038	-0.014	0.016
108.931	197.164	60.514	0.004	-0.014	0.057
60.513	60.514	601.975	-0.003	-0.006	0.030
-0.038	0.004	-0.003	176.646	0.002	0.004
-0.014	-0.014	-0.006	0.002	176.603	-0.011
0.016	0.057	0.030	0.004	-0.011	87.140

BN-141

Density (g/cm^3): 2.57 | Space Group: 38

Bulk modulus (GPa): 252 | Shear modulus (GPa): 173

Young's modulus (GPa): 422 | Highest Young's modulus (GPa): 906

Hardness (GPa): 23 | Energy above hull (eV/atom): 0.15

Primitive Cell

1.000000

2.50948936204910	0.00000000000000	0.00000000000000
0.00000000000000	3.03296009367075	3.16268857200749
0.00000000000000	-3.03296009367075	3.16268857200749

B N

3 3

DIRECT

0.5000000000000000	0.9238002311393183	0.9238002311393183
0.0000000000000000	0.0154879286928688	0.4185088879553864
0.0000000000000000	0.4185088879553864	0.0154879286928688
0.0000000000000000	0.0718560811477819	0.0718560811477818
0.5000000000000000	0.9950503704763816	0.5752964319781078
0.5000000000000000	0.5752964319781078	0.9950503704763816

Stiffness tensor (GPa):

928.255	92.815	66.275	-0.049	0.032	0.044
92.815	405.229	231.878	-0.022	0.001	0.043
66.275	231.878	290.588	-0.030	0.004	0.058
-0.049	-0.022	-0.030	221.503	-0.003	0.022
0.032	0.001	0.004	-0.003	189.559	-0.003
0.044	0.043	0.058	0.022	-0.003	209.167

BN-142

Density (g/cm^3): 2.57	Space Group: 136
Bulk modulus (GPa): 177	Shear modulus (GPa): 128
Young's modulus (GPa): 309	Highest Young's modulus (GPa): 483
Hardness (GPa): 20	Energy above hull (eV/atom): 0.76

Primitive Cell

1.000000

4.90596459431662	0.00000000000000	0.00000000000000
0.00000000000000	4.90596459431662	0.00000000000000
0.00000000000000	0.00000000000000	8.00628688888477

B N

12 12

DIRECT

0.3384182737414704	0.3384182737414704	0.3085006375663346
0.6615817262585296	0.6615817262585296	0.6914993624336654
0.6615817262585296	0.6615817262585296	0.3085006375663346
0.3384182737414704	0.3384182737414704	0.6914993624336654
0.1615817262585296	0.8384182737414704	0.8085006375663346
0.8384182737414704	0.1615817262585296	0.1914993624336654
0.8384182737414704	0.1615817262585296	0.8085006375663346
0.1615817262585296	0.8384182737414704	0.1914993624336654
0.8582537719171041	0.8582537719171041	0.0000000000000000
0.1417462280828959	0.1417462280828959	0.0000000000000000
0.6417462280828959	0.3582537719171039	0.5000000000000000
0.3582537719171039	0.6417462280828959	0.5000000000000000
0.6727850834276874	0.3272149165723127	0.3057363553189087
0.3272149165723126	0.6727850834276874	0.6942636446810913
0.3272149165723126	0.6727850834276874	0.3057363553189087
0.6727850834276874	0.3272149165723127	0.6942636446810913
0.8272149165723126	0.8272149165723126	0.8057363553189087
0.1727850834276873	0.1727850834276874	0.1942636446810913
0.1727850834276873	0.1727850834276874	0.8057363553189087
0.8272149165723126	0.8272149165723126	0.1942636446810913
0.1823340545340432	0.8176659454659568	0.0000000000000000
0.8176659454659568	0.1823340545340432	0.0000000000000000
0.3176659454659569	0.3176659454659568	0.5000000000000000
0.6823340545340432	0.6823340545340432	0.5000000000000000

Stiffness tensor (GPa):

205.764	103.646	148.654	-0.019	-0.020	0.007
103.646	205.840	148.692	-0.012	-0.018	-0.002
148.654	148.692	581.485	-0.028	-0.017	0.009
-0.019	-0.012	-0.028	197.212	0.007	-0.005
-0.020	-0.018	-0.017	0.007	197.209	0.001
0.007	-0.002	0.009	-0.005	0.001	137.718

BN-143

Density (g/cm^3): 2.55 | Space Group: 5

Bulk modulus (GPa): 209 | Shear modulus (GPa): 107

Young's modulus (GPa): 275 | Highest Young's modulus (GPa): 452

Hardness (GPa): 11 | Energy above hull (eV/atom): 0.39

Primitive Cell

```
  1.000000
     4.49015091904227    -1.59580710221516     0.00000000000000
     4.49015091904227     1.59580710221516     0.00000000000000
    -4.49014234987721     0.00000000000000     4.50430530873952
  B     N
  4     4
DIRECT
     0.9999189737854293    0.5000366249472887    0.6338845368688644
     0.4999633750527113    0.0000810262145708    0.3661154631311357
     0.8838467862999454    0.8839655588895330    0.1338839985392335
     0.1160344411104669    0.1161532137000545    0.8661160014607665
     0.0004540652329586    0.5003357659170429    0.8546627472434003
     0.4996642340829570    0.9995459347670413    0.1453372527565997
     0.1043283971081180    0.1042091880238308    0.3546636890043642
     0.8957908119761692    0.8956716028918820    0.6453363109956358
```

Stiffness tensor (GPa):

473.727	302.170	175.487	0.003	0.043	0.011
302.170	480.746	176.830	0.013	-0.016	0.047
175.487	176.830	151.838	0.036	0.030	0.042
0.003	0.013	0.036	142.191	0.011	0.011
0.043	-0.016	0.030	0.011	134.832	0.031
0.011	0.047	0.042	0.011	0.031	222.982

BN-144

Density (g/cm^3): 2.55 | Space Group: 127

Bulk modulus (GPa): 248 | Shear modulus (GPa): 170

Young's modulus (GPa): 415 | Highest Young's modulus (GPa): 900

Hardness (GPa): 23 | Energy above hull (eV/atom): 0.17

Primitive Cell

1.000000

8.79143937667008	0.00000000000000	0.00000000000000
0.00000000000000	8.79143937667008	0.00000000000000
0.00000000000000	0.00000000000000	2.51096629261581

B N

12 12

DIRECT

0.4548765068494842	0.7642422361812591	0.0000000000000000
0.5451234931505158	0.2357577638187409	0.0000000000000000
0.2642422361812591	0.9548765068494842	0.0000000000000000
0.7357577638187409	0.0451234931505158	0.0000000000000000
0.2928747052844325	0.2071252947155675	0.5000000000000000
0.7071252947155675	0.7928747052844325	0.5000000000000000
0.2357577638187409	0.4548765068494842	0.0000000000000000
0.7642422361812591	0.5451234931505158	0.0000000000000000
0.0451234931505158	0.2642422361812591	0.0000000000000000
0.9548765068494842	0.7357577638187409	0.0000000000000000
0.2071252947155675	0.7071252947155675	0.5000000000000000
0.7928747052844325	0.2928747052844325	0.5000000000000000
0.7364491264552107	0.9667550437326060	0.5000000000000000
0.2635508735447893	0.0332449562673940	0.5000000000000000
0.5332449562673940	0.7635508735447893	0.5000000000000000
0.4667550437326060	0.2364491264552107	0.5000000000000000
0.7185994702542740	0.2185994702542740	0.0000000000000000
0.2814005297457260	0.7814005297457260	0.0000000000000000
0.9667550437326060	0.2635508735447893	0.5000000000000000
0.0332449562673940	0.7364491264552107	0.5000000000000000
0.7635508735447893	0.4667550437326060	0.5000000000000000
0.2364491264552107	0.5332449562673940	0.5000000000000000
0.7814005297457260	0.7185994702542740	0.0000000000000000
0.2185994702542740	0.2814005297457260	0.0000000000000000

Stiffness tensor (GPa):

460.284	84.904	79.476	0.013	-0.017	0.014
84.904	460.310	79.532	0.008	0.017	0.014
79.476	79.532	923.582	0.011	0.005	0.021
0.013	0.008	0.011	201.153	0.004	0.005
-0.017	0.017	0.005	0.004	201.186	0.006
0.014	0.014	0.021	0.005	0.006	58.807

BN-145

Density (g/cm^3): 2.50 | Space Group: 105

Bulk modulus (GPa): 254 | Shear modulus (GPa): 147

Young's modulus (GPa): 371 | Highest Young's modulus (GPa): 775

Hardness (GPa): 17 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.81956195478355	0.00000000000000	0.00000000000000
0.00000000000000	4.81956195478355	0.00000000000000
0.00000000000000	0.00000000000000	4.25638161643217

B N

6 6

DIRECT

0.0000000000000000	0.5000000000000000	0.3385440831831086
0.5000000000000000	0.0000000000000000	0.8385440831831086
0.7212173729287559	0.5000000000000000	0.8162510817760776
0.2787826270712442	0.5000000000000000	0.8162510817760776
0.5000000000000000	0.7212173729287559	0.3162510817760777
0.5000000000000000	0.2787826270712442	0.3162510817760777
0.0000000000000000	0.5000000000000000	0.6680650287943409
0.5000000000000000	0.0000000000000000	0.1680650287943410
0.2689414036081323	0.5000000000000000	0.1804443582228061
0.7310585963918677	0.5000000000000000	0.1804443582228061
0.5000000000000000	0.2689414036081323	0.6804443582228061
0.5000000000000000	0.7310585963918677	0.6804443582228061

Stiffness tensor (GPa):

584.787	31.574	73.699	0.009	0.011	-0.021
31.574	584.767	73.736	0.012	-0.022	0.050
73.699	73.736	792.301	0.012	0.017	0.040
0.009	0.012	0.012	210.267	0.003	0.002
0.011	-0.022	0.017	0.003	210.275	0.000
-0.021	0.050	0.040	0.002	0.000	24.302

BN-146

Density (g/cm^3): 2.50 | Space Group: 121
Bulk modulus (GPa): 130 | Shear modulus (GPa): 103
Young's modulus (GPa): 245 | Highest Young's modulus (GPa): 448
Hardness (GPa): 20 | Energy above hull (eV/atom): 0.93

Primitive Cell

1.000000

-2.44859745627189	2.44859745627189	5.50144553089421
2.44859745627189	-2.44859745627189	5.50144553089421
2.44859745627189	2.44859745627189	-5.50144553089421

B N

8 8

DIRECT

0.0445562142189060	0.0445562142189060	0.6755313107081657
0.3690249035107402	0.3690249035107402	0.3244686892918343
0.9554437857810940	0.6309750964892598	0.0000000000000000
0.6309750964892598	0.9554437857810940	0.0000000000000000
0.0792359784006521	0.0792359784006521	0.2941383968698301
0.7850975815308219	0.7850975815308219	0.7058616031301699
0.9207640215993480	0.2149024184691781	0.0000000000000000
0.2149024184691781	0.9207640215993480	0.0000000000000000
0.9632894438123074	0.9632894438123074	0.3451690517821654
0.6181203920301419	0.6181203920301419	0.6548309482178345
0.0367105561876926	0.3818796079698581	0.0000000000000000
0.3818796079698581	0.0367105561876926	0.0000000000000000
0.8814161509350313	0.8814161509350313	0.6281417902753965
0.2532743606596348	0.2532743606596348	0.3718582097246035
0.1185838490649687	0.7467256393403652	0.0000000000000000
0.7467256393403652	0.1185838490649687	0.0000000000000000

Stiffness tensor (GPa):

151.460	62.921	100.420	0.181	0.041	-0.046
62.921	151.458	100.423	0.026	0.177	-0.031
100.420	100.423	541.717	0.078	0.069	0.012
0.181	0.026	0.078	141.398	0.004	-0.020
0.041	0.177	0.069	0.004	141.356	-0.018
-0.046	-0.031	0.012	-0.020	-0.018	106.097

BN-147

Density (g/cm^3): 2.40
Space Group: 145
Bulk modulus (GPa): 229
Shear modulus (GPa): 167
Young's modulus (GPa): 404
Highest Young's modulus (GPa): 829
Hardness (GPa): 25
Energy above hull (eV/atom): 0.20

Primitive Cell

1.000000

8.44762863197627	0.00000000000000	0.00000000000000
-4.22381431598814	7.31586099702824	0.00000000000000
0.00000000000000	0.00000000000000	2.50246553866597

B N

9 9

DIRECT

0.6380880056943710	0.4716520724139315	0.9030902014757279
0.2502438487538171	0.9221201691182871	0.1520685623226775
0.6652510488643080	0.0043591929202417	0.0310097354875145
0.6718763203644700	0.7497561512461829	0.4854018956560108
0.8335640667195607	0.3619119943056291	0.2364235348090613
0.5283479275860685	0.1664359332804394	0.5697568681423946
0.3391081440559338	0.3347489511356921	0.3643430688208478
0.9956408070797583	0.6608918559440662	0.6976764021541811
0.0778798308817129	0.3281236796355300	0.8187352289893441
0.6673658737741206	0.6628099770362677	0.9773713051093690
0.6731200872274781	0.9237863297193400	0.5221114766688418
0.0762136702806599	0.7493337575081379	0.1887781433355085
0.6403713630782866	0.1679253204492449	0.0810153243148705
0.8320746795507552	0.4724460426290416	0.7476819909815371
0.3371900229637323	0.0045558967378528	0.6440379717760356
0.9954441032621472	0.3326341262258795	0.3107046384427024
0.2506662424918620	0.3268799127725220	0.8554448100021752
0.5275539573709584	0.3596286369217135	0.4143486576482038

Stiffness tensor (GPa):

379.799	133.045	67.184	14.389	4.862	0.021
133.045	379.074	67.219	-14.303	-4.739	-0.166
67.184	67.219	846.411	-0.051	0.033	0.136
14.389	-14.303	-0.051	164.089	-0.011	-4.820
4.862	-4.739	0.033	-0.011	164.117	14.409
0.021	-0.166	0.136	-4.820	14.409	122.740

BN-148

Density (g/cm^3): 2.36 | Space Group: 122
Bulk modulus (GPa): 210 | Shear modulus (GPa): 81
Young's modulus (GPa): 216 | Highest Young's modulus (GPa): 375
Hardness (GPa): 6 | Energy above hull (eV/atom): 0.33

Primitive Cell

1.000000

-3.02509946243983	3.02509946243983	1.90746244281622
3.02509946243983	-3.02509946243983	1.90746244281622
3.02509946243983	3.02509946243983	-1.90746244281622

B N

4 4

DIRECT

0.9933952737244065	0.1250000000000000	0.3683952737244065
0.7566047262755935	0.6250000000000000	0.6316047262755935
0.3750000000000000	0.0066047262755935	0.1316047262755935
0.8750000000000000	0.2433952737244065	0.8683952737244065
0.7613204283912163	0.1250000000000000	0.1363204283912163
0.9886795716087837	0.6250000000000000	0.8636795716087837
0.3750000000000000	0.2386795716087837	0.3636795716087837
0.8750000000000000	0.0113204283912163	0.6363204283912163

Stiffness tensor (GPa):

444.492	139.461	204.838	-0.033	0.026	0.026
139.461	444.424	204.835	0.009	-0.017	0.032
204.838	204.835	184.452	0.044	0.019	0.057
-0.033	0.009	0.044	147.645	0.020	0.013
0.026	-0.017	0.019	0.020	147.660	0.013
0.026	0.032	0.057	0.013	0.013	76.895

BN-149

Density (g/cm^3): 2.36
Space Group: 160
Bulk modulus (GPa): 227
Shear modulus (GPa): 149
Young's modulus (GPa): 367
Highest Young's modulus (GPa): 747
Hardness (GPa): 20
Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

7.33458938721708	4.23462715710515	0.84322042639615
-7.33458938721708	4.23462715710515	0.84322042639615
0.00000000000000	-8.46925431421031	0.84322042639615

B N

9 9

DIRECT

0.5850551470963755	0.3844279724816491	0.5850551470963756
0.3844279724816491	0.5850551470963756	0.5850551470963756
0.5850551470963755	0.5850551470963755	0.3844279724816491
0.8758335054209166	0.8758335054209166	0.1562709400891293
0.8758335054209166	0.1562709400891293	0.8758335054209168
0.1562709400891292	0.8758335054209168	0.8758335054209168
0.2313514913181124	0.2313514913181124	0.7670087761901270
0.2313514913181124	0.7670087761901270	0.2313514913181126
0.7670087761901270	0.2313514913181125	0.2313514913181126
0.4215643436367718	0.6063303748764419	0.4215643436367719
0.6063303748764418	0.4215643436367720	0.4215643436367719
0.4215643436367718	0.4215643436367718	0.6063303748764418
0.1306379337422846	0.1306379337422846	0.8330817285685391
0.1306379337422846	0.8330817285685389	0.1306379337422848
0.8330817285685389	0.1306379337422847	0.1306379337422848
0.7722564853889686	0.7722564853889686	0.2194825951344060
0.7722564853889686	0.2194825951344061	0.7722564853889686
0.2194825951344060	0.7722564853889686	0.7722564853889686

Stiffness tensor (GPa):

348.684	155.672	84.027	5.370	-0.000	-0.076
155.672	348.388	84.594	-5.352	0.005	0.002
84.027	84.594	775.134	0.024	0.007	0.009
5.370	-5.352	0.024	166.242	0.000	0.041
-0.000	0.005	0.007	0.000	166.290	5.327
-0.076	0.002	0.009	0.041	5.327	95.646

BN-150

Density (g/cm^3): 2.34
Space Group: 35
Bulk modulus (GPa): 221
Shear modulus (GPa): 174
Young's modulus (GPa): 413
Highest Young's modulus (GPa): 670
Hardness (GPa): 28
Energy above hull (eV/atom): 0.48

Primitive Cell

1.000000

2.44519733911458	-4.23530187608384	0.00000000000000
2.44519733911458	4.23530187608384	0.00000000000000
0.00000000000000	0.00000000000000	4.24680991936800

B N

5 5

DIRECT

0.6666646116048597	0.3333353883951403	0.1949487708842632
0.3333353883951403	0.6666646116048597	0.1949487708842632
0.5000000000000000	0.5000000000000000	0.6548824590707834
0.0000000000000000	0.5000000000000000	0.6548812689764592
0.5000000000000000	0.0000000000000000	0.6548812689764592
0.6666645597065199	0.3333354402934801	0.8219781217517872
0.3333354402934801	0.6666645597065199	0.8219781217517872
0.5000000000000000	0.5000000000000000	0.3338327503676930
0.0000000000000000	0.5000000000000000	0.3338342365322876
0.5000000000000000	0.0000000000000000	0.3338342365322876

Stiffness tensor (GPa):

399.953	142.496	60.580	0.147	-0.032	0.008
142.496	399.684	60.493	-0.033	-0.013	-0.018
60.580	60.493	683.947	0.040	0.005	0.017
0.147	-0.033	0.040	185.639	0.003	0.011
-0.032	-0.013	0.005	0.003	185.572	-0.005
0.008	-0.018	0.017	0.011	-0.005	128.210

BN-151

Density (g/cm^3): 2.31 | Space Group: 127

Bulk modulus (GPa): 230 | Shear modulus (GPa): 83

Young's modulus (GPa): 222 | Highest Young's modulus (GPa): 736

Hardness (GPa): 5 | Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

7.49819047000565	0.00000000000000	0.00000000000000
0.00000000000000	7.49819047000565	0.00000000000000
0.00000000000000	0.00000000000000	2.53425391409489

B N

8 8

DIRECT

0.6060848539529496	0.1060848539529497	0.0000000000000000
0.3939151460470504	0.8939151460470502	0.0000000000000000
0.8939151460470502	0.6060848539529496	0.0000000000000000
0.1060848539529497	0.3939151460470504	0.0000000000000000
0.3121484861590951	0.1878515138409050	0.5000000000000000
0.6878515138409049	0.8121484861590951	0.5000000000000000
0.8121484861590951	0.3121484861590951	0.5000000000000000
0.1878515138409050	0.6878515138409049	0.5000000000000000
0.1138463955173509	0.6138463955173508	0.0000000000000000
0.8861536044826491	0.3861536044826492	0.0000000000000000
0.3861536044826492	0.1138463955173509	0.0000000000000000
0.6138463955173508	0.8861536044826491	0.0000000000000000
0.8195128604348565	0.6804871395651435	0.5000000000000000
0.1804871395651435	0.3195128604348565	0.5000000000000000
0.3195128604348565	0.8195128604348565	0.5000000000000000
0.6804871395651435	0.1804871395651435	0.5000000000000000

Stiffness tensor (GPa):

255.950	254.766	87.399	0.021	0.007	0.059
254.766	256.143	87.174	0.009	-0.001	-0.068
87.399	87.174	766.335	0.004	0.004	-0.011
0.021	0.009	0.004	180.884	0.002	0.013
0.007	-0.001	0.004	0.002	180.914	0.007
0.059	-0.068	-0.011	0.013	0.007	167.311

BN-152

Density (g/cm^3): 2.29 | Space Group: 211

Bulk modulus (GPa): 229 | Shear modulus (GPa): 135

Young's modulus (GPa): 338 | Highest Young's modulus (GPa): 470

Hardness (GPa): 16 | Energy above hull (eV/atom): 0.65

Primitive Cell

1.000000

-3.77975499269292	3.77975499269292	3.77975499269292
3.77975499269292	-3.77975499269292	3.77975499269292
3.77975499269292	3.77975499269292	-3.77975499269292

B N

12 12

DIRECT

0.1470182959081090	0.2940365918162179	0.6470182959081090
0.6470182959081090	0.5000000000000000	0.3529817040918910
0.3529817040918910	0.7059634081837820	0.8529817040918910
0.8529817040918910	0.5000000000000000	0.1470182959081090
0.6470182959081090	0.1470182959081090	0.2940365918162179
0.3529817040918910	0.6470182959081090	0.5000000000000000
0.8529817040918910	0.3529817040918910	0.7059634081837820
0.1470182959081090	0.8529817040918910	0.5000000000000000
0.2940365918162179	0.6470182959081090	0.1470182959081090
0.5000000000000000	0.3529817040918910	0.6470182959081090
0.7059634081837820	0.8529817040918910	0.3529817040918910
0.5000000000000000	0.1470182959081090	0.8529817040918910
0.8602017067510848	0.7204034135021694	0.3602017067510846
0.3602017067510846	0.5000000000000000	0.6397982932489154
0.6397982932489154	0.2795965864978306	0.1397982932489153
0.1397982932489153	0.5000000000000000	0.8602017067510848
0.3602017067510848	0.8602017067510846	0.7204034135021694
0.6397982932489152	0.3602017067510848	0.5000000000000000
0.1397982932489154	0.6397982932489152	0.2795965864978306
0.8602017067510846	0.1397982932489154	0.5000000000000000
0.7204034135021694	0.3602017067510846	0.8602017067510848
0.5000000000000000	0.6397982932489154	0.3602017067510846
0.2795965864978306	0.1397982932489153	0.6397982932489154
0.5000000000000000	0.8602017067510848	0.1397982932489153

Stiffness tensor (GPa):

325.880	180.226	180.223	-0.015	0.022	-0.006
180.226	325.868	180.228	-0.011	0.006	0.030
180.223	180.228	325.891	0.012	-0.039	-0.001
-0.015	-0.011	0.012	203.119	0.001	-0.003
0.022	0.006	-0.039	0.001	203.110	-0.004
-0.006	0.030	-0.001	-0.003	-0.004	203.125

BN-153

Density (g/cm^3): 2.29 | Space Group: 15

Bulk modulus (GPa): 207 | Shear modulus (GPa): 55

Young's modulus (GPa): 151 | Highest Young's modulus (GPa): 414

Hardness (GPa): 1 | Energy above hull (eV/atom): 0.34

Primitive Cell

1.000000

3.21060567942271	-3.55295916321621	0.00000000000000
3.21060567942271	3.55295916321621	0.00000000000000
-0.72119323544688	0.00000000000000	4.73406590468502

B N

6 6

DIRECT

0.3443146249008369	0.6556853750991631	0.2500000000000000
0.6556853750991631	0.3443146249008369	0.7500000000000000
0.1556852870934535	0.2500000704817014	0.8443146157284178
0.8443147129065465	0.7499999295182986	0.1556853842715822
0.7499999295182986	0.8443147129065465	0.6556853842715822
0.2500000704817014	0.1556852870934535	0.3443146157284178
0.8547091348444291	0.1452908651555709	0.7500000000000000
0.1452908651555709	0.8547091348444291	0.2500000000000000
0.6452907048797066	0.7500000979542811	0.3547093096512224
0.3547092951202934	0.2499999020457189	0.6452906903487776
0.2499999020457189	0.3547092951202933	0.1452906903487776
0.7500000979542811	0.6452907048797067	0.8547093096512224

Stiffness tensor (GPa):

213.259	155.422	183.005	50.219	0.017	0.017
155.422	213.147	182.828	-50.400	-0.011	0.025
183.005	182.828	595.593	0.120	0.022	0.038
50.219	-50.400	0.120	129.511	0.023	0.022
0.017	-0.011	0.022	0.023	129.141	50.223
0.017	0.025	0.038	0.022	50.223	28.915

BN-154

Density (g/cm^3): 2.27 | Space Group: 132

Bulk modulus (GPa): 230 | Shear modulus (GPa): 74

Young's modulus (GPa): 199 | Highest Young's modulus (GPa): 589

Hardness (GPa): 4 | Energy above hull (eV/atom): 0.49

Primitive Cell

1.000000

4.92448975819440	0.00000000000000	0.00000000000000
0.00000000000000	4.92448975819440	0.00000000000000
0.00000000000000	0.00000000000000	4.48434233115922

B N

6 6

DIRECT

0.0000000000000000	0.0000000000000000	0.2500000000000000
0.0000000000000000	0.0000000000000000	0.7500000000000000
0.6493090509395953	0.3506909490604047	0.0000000000000000
0.3506909490604047	0.6493090509395953	0.0000000000000000
0.6493090509395953	0.6493090509395953	0.5000000000000000
0.3506909490604047	0.3506909490604047	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.2500000000000000
0.5000000000000000	0.5000000000000000	0.7500000000000000
0.1572217158501489	0.8427782841498511	0.0000000000000000
0.8427782841498511	0.1572217158501489	0.0000000000000000
0.1572217158501489	0.1572217158501489	0.5000000000000000
0.8427782841498511	0.8427782841498511	0.5000000000000000

Stiffness tensor (GPa):

289.568	264.889	89.033	0.012	0.021	-0.000
264.889	289.583	89.033	0.011	0.024	-0.016
89.033	89.033	617.489	0.029	0.020	-0.013
0.012	0.011	0.029	33.649	0.018	-0.044
0.021	0.024	0.020	0.018	33.636	-0.004
-0.000	-0.016	-0.013	-0.044	-0.004	249.168

BN-155

Density (g/cm^3): 2.25	Space Group: 4
Bulk modulus (GPa): 178	Shear modulus (GPa): 84
Young's modulus (GPa): 218	Highest Young's modulus (GPa): 472
Hardness (GPa): 8	Energy above hull (eV/atom): 0.26

Primitive Cell

1.000000

4.93121488820555	0.00000000000000	0.00000000000000
0.00000000000000	4.52037706567014	0.00000000000000
-0.20734879820990	0.00000000000000	4.93289998610476

B N

6 6

DIRECT

0.6107967405704524	0.1088855698283089	0.5316829962675106
0.3892032594295476	0.6088855698283089	0.4683170037324894
0.0272409907730341	0.4029882065477782	0.1166137476084297
0.9727590092269659	0.9029882065477782	0.8833862523915703
0.0913693841876228	0.9291182402338449	0.3891229150710287
0.9086306158123771	0.4291182402338449	0.6108770849289713
0.9771989229193899	0.5809438606450937	0.8796394259911675
0.0228010770806101	0.0809438606450938	0.1203605740088325
0.9119716086807835	0.0602085955150007	0.6176000964618591
0.0880283913192165	0.5602085955150007	0.3823999035381409
0.3930053311629665	0.9178556002936297	0.4826173521138344
0.6069946688370336	0.4178556002936298	0.5173826478861656

Stiffness tensor (GPa):

297.889	162.399	128.920	-0.001	47.867	0.070
162.399	561.757	98.331	-0.025	24.704	0.042
128.920	98.331	382.760	-0.008	32.383	-0.037
-0.001	-0.025	-0.008	174.152	0.032	49.010
47.867	24.704	32.383	0.032	19.289	0.060
0.070	0.042	-0.037	49.010	0.060	157.378

BN-156

Density (g/cm^3): 2.21 | Space Group: 185
Bulk modulus (GPa): 221 | Shear modulus (GPa): 158
Young's modulus (GPa): 383 | Highest Young's modulus (GPa): 717
Hardness (GPa): 23 | Energy above hull (eV/atom): 0.10

Primitive Cell

1.000000

9.49165855532529	0.00000000000000	0.00000000000000
-4.74582927766265	8.22001743295961	0.00000000000000
0.00000000000000	0.00000000000000	4.30588844846676

B N

18 18

DIRECT

0.0000000000000000	0.4341606348236291	0.5819625763517656
0.5658393651763709	0.5658393651763709	0.5819625763517656
0.4341606348236290	0.0000000000000000	0.5819625763517656
-0.0000000000000000	0.5658393651763709	0.0819625763517658
0.4341606348236290	0.4341606348236291	0.0819625763517658
0.5658393651763710	0.0000000000000000	0.0819625763517658
0.3024936499236430	0.3024936499236430	0.5860839274060884
0.6975063500763570	0.0000000000000000	0.5860839274060884
-0.0000000000000000	0.6975063500763570	0.5860839274060884
0.6975063500763570	0.6975063500763570	0.0860839274060885
0.3024936499236430	0.0000000000000000	0.0860839274060885
0.0000000000000000	0.3024936499236430	0.0860839274060885
0.8409371920565967	0.8409371920565967	0.5637731343305635
0.1590628079434033	0.0000000000000000	0.5637731343305635
0.0000000000000000	0.1590628079434034	0.5637731343305635
0.1590628079434034	0.1590628079434034	0.0637731343305637
0.8409371920565967	0.0000000000000000	0.0637731343305637
-0.0000000000000000	0.8409371920565967	0.0637731343305637
-0.0000000000000000	0.5672675279199495	0.4166407107113919
0.4327324720800504	0.4327324720800505	0.4166407107113919
0.5672675279199496	0.0000000000000000	0.4166407107113919
0.0000000000000000	0.4327324720800505	0.9166407107113917
0.5672675279199495	0.5672675279199495	0.9166407107113917
0.4327324720800504	0.0000000000000000	0.9166407107113917
0.6961790125184368	0.6961790125184368	0.4162959855358621
0.3038209874815632	0.0000000000000000	0.4162959855358621
0.0000000000000000	0.3038209874815632	0.4162959855358621
0.3038209874815632	0.3038209874815632	0.9162959855358620
0.6961790125184368	0.0000000000000000	0.9162959855358620
-0.0000000000000000	0.6961790125184368	0.9162959855358620
0.1575010133240255	0.1575010133240255	0.4352436595614980
0.8424989866759746	0.0000000000000000	0.4352436595614980
-0.0000000000000000	0.8424989866759746	0.4352436595614980

0.8424989866759746	0.8424989866759746	0.9352436595614979
0.1575010133240254	0.0000000000000000	0.9352436595614979
0.0000000000000000	0.1575010133240255	0.9352436595614979

Stiffness tensor (GPa):

360.845	143.521	74.919	0.016	-0.001	-0.076
143.521	361.571	75.686	-0.003	0.001	0.032
74.919	75.686	739.794	-0.021	0.001	0.037
0.016	-0.003	-0.021	172.945	0.002	0.019
-0.001	0.001	0.001	0.002	173.001	-0.009
-0.076	0.032	0.037	0.019	-0.009	106.755

BN-157

Density (g/cm^3): 2.18 | Space Group: 36
Bulk modulus (GPa): 216 | Shear modulus (GPa): 150
Young's modulus (GPa): 366 | Highest Young's modulus (GPa): 646
Hardness (GPa): 21 | Energy above hull (eV/atom): 0.15

Primitive Cell

1.000000

8.19540908449490	-4.77932236666519	0.00000000000000
8.19540908449490	4.77932236666519	0.00000000000000
0.00000000000000	0.00000000000000	4.34922013081715

B N

18 18

DIRECT

0.3401865099761381	0.5001384300387974	0.0704568678023065
0.6598134900238619	0.4998615699612026	0.5704568678023065
0.5001384300387974	0.3401865099761381	0.5704568678023065
0.4998615699612026	0.6598134900238619	0.0704568678023065
0.8033000212401291	0.4996502556248326	0.0924709817395373
0.1966999787598709	0.5003497443751674	0.5924709817395373
0.4996502556248326	0.8033000212401291	0.5924709817395373
0.5003497443751674	0.1966999787598709	0.0924709817395373
0.0659199350352244	0.4999391890643006	0.0880380379898973
0.9340800649647756	0.5000608109356994	0.5880380379898973
0.4999391890643006	0.0659199350352244	0.5880380379898973
0.5000608109356994	0.9340800649647756	0.0880380379898973
0.9347711809278174	0.0652288190721826	0.8960437779127872
0.0652288190721826	0.9347711809278174	0.3960437779127872
0.8072154122524811	0.1927845877475189	0.3905630825564108
0.1927845877475189	0.8072154122524811	0.8905630825564108
0.6505628487478436	0.3494371512521564	0.0675224717241339
0.3494371512521564	0.6505628487478436	0.5675224717241339
0.6590419933574245	0.4999182165641867	0.9393133071407958
0.3409580066425755	0.5000817834358133	0.4393133071407958
0.4999182165641867	0.6590419933574245	0.4393133071407958
0.5000817834358133	0.3409580066425755	0.9393133071407958
0.1959869285954068	0.4998118197375407	0.9213551097929475
0.8040130714045932	0.5001881802624593	0.4213551097929475
0.4998118197375407	0.1959869285954068	0.4213551097929475
0.5001881802624593	0.8040130714045932	0.9213551097929475
0.9329163601192270	0.5000021055672135	0.9218384080992545
0.0670836398807729	0.4999978944327866	0.4218384080992545
0.5000021055672134	0.9329163601192271	0.4218384080992545
0.4999978944327866	0.0670836398807730	0.9218384080992545
0.0666206157990317	0.9333793842009683	0.0661570964555852
0.9333793842009683	0.0666206157990317	0.5661570964555851
0.1912326524374770	0.8087673475625230	0.5671167381005242

0.8087673475625230	0.1912326524374770	0.0671167381005242
0.3512944159278767	0.6487055840721232	0.9456514072021656
0.6487055840721233	0.3512944159278767	0.4456514072021656

Stiffness tensor (GPa):

359.990	143.266	75.595	0.002	-0.002	0.037
143.266	339.153	89.747	0.031	0.005	-0.052
75.595	89.747	674.378	0.012	0.007	0.014
0.002	0.031	0.012	159.868	0.008	-0.006
-0.002	0.005	0.007	0.008	173.550	-0.008
0.037	-0.052	0.014	-0.006	-0.008	105.614

BN-158

Density (g/cm^3): 2.11 Space Group: 185

Bulk modulus (GPa): 210 Shear modulus (GPa): 133

Young's modulus (GPa): 330 Highest Young's modulus (GPa): 521

Hardness (GPa): 18 Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

9.54421880616955	0.00000000000000	0.00000000000000
-4.77210940308477	8.26553594542001	0.00000000000000
0.00000000000000	0.00000000000000	4.45775974582391

B N

18 18

DIRECT

0.0000000000000000	0.8483221376301351	0.9175249738324708
0.1516778623698649	0.1516778623698649	0.9175249738324708
0.8483221376301351	0.0000000000000000	0.9175249738324708
0.0000000000000000	0.1516778623698649	0.4175249738324708
0.8483221376301351	0.8483221376301351	0.4175249738324708
0.1516778623698649	0.0000000000000000	0.4175249738324708
0.0000000000000000	0.3090231502037397	0.1005372234951474
0.6909768497962603	0.6909768497962603	0.1005372234951474
0.3090231502037397	0.0000000000000000	0.1005372234951474
0.0000000000000000	0.6909768497962603	0.6005372234951474
0.3090231502037397	0.3090231502037397	0.6005372234951474
0.6909768497962603	0.0000000000000000	0.6005372234951474
0.0000000000000000	0.5652571609609283	0.0935929029001741
0.4347428390390717	0.4347428390390717	0.0935929029001741
0.5652571609609283	0.0000000000000000	0.0935929029001741
0.0000000000000000	0.4347428390390717	0.5935929029001741
0.5652571609609283	0.5652571609609283	0.5935929029001741
0.4347428390390717	0.0000000000000000	0.5935929029001741
0.0000000000000000	0.1511061054753912	0.0478763214858890
0.8488938945246087	0.8488938945246087	0.0478763214858890
0.1511061054753912	0.0000000000000000	0.0478763214858890
0.0000000000000000	0.8488938945246087	0.5478763214858891
0.1511061054753912	0.1511061054753912	0.5478763214858891
0.8488938945246087	0.0000000000000000	0.5478763214858891
0.0000000000000000	0.6898666662718920	0.9191857320271849
0.3101333337281081	0.3101333337281081	0.9191857320271849
0.6898666662718920	0.0000000000000000	0.9191857320271849
0.0000000000000000	0.3101333337281081	0.4191857320271847
0.6898666662718920	0.6898666662718920	0.4191857320271847
0.3101333337281081	0.0000000000000000	0.4191857320271847
0.0000000000000000	0.4335208951807202	0.9212828470586107
0.5664791048192797	0.5664791048192797	0.9212828470586107
0.4335208951807203	0.0000000000000000	0.9212828470586107

0.0000000000000000	0.5664791048192797	0.4212828470586107
0.4335208951807202	0.4335208951807203	0.4212828470586107
0.5664791048192797	0.0000000000000000	0.4212828470586107

Stiffness tensor (GPa):

337.318	139.539	98.898	0.028	-0.025	-0.084
139.539	337.701	99.807	-0.050	0.019	-0.005
98.898	99.807	562.321	-0.036	0.001	0.032
0.028	-0.050	-0.036	148.638	0.001	0.010
-0.025	0.019	0.001	0.001	148.600	-0.032
-0.084	-0.005	0.032	0.010	-0.032	96.801

BN-159

Density (g/cm^3): 2.01
Space Group: 44
Bulk modulus (GPa): 187
Shear modulus (GPa): 88
Young's modulus (GPa): 228
Highest Young's modulus (GPa): 703
Hardness (GPa): 8
Energy above hull (eV/atom): 0.24

Primitive Cell

1.000000

-1.26247065616588	3.05833426211426	5.29849286421458
1.26247065616588	-3.05833426211426	5.29849286421458
1.26247065616588	3.05833426211426	-5.29849286421458

B N

4 4

DIRECT

0.8564223172199885	0.8564223172199885	0.0000000000000000
0.4360957998251105	0.2318138441636635	0.2042819556614470
0.0275318885022164	0.2318138441636635	0.7957180443385530
0.0640809534411869	0.5640809534411870	0.5000000000000000
0.1434693180250408	0.1434693180250408	0.0000000000000000
0.5594675288985487	0.7682921714849251	0.7911753574136235
0.9771168140713016	0.7682921714849251	0.2088246425863765
0.9358153757077345	0.4358153757077345	0.5000000000000000

Stiffness tensor (GPa):

728.695	59.119	84.569	0.020	-0.002	0.019
59.119	196.152	170.062	0.019	-0.026	0.030
84.569	170.062	284.241	0.061	0.010	0.031
0.020	0.019	0.061	22.026	-0.007	0.031
-0.002	-0.026	0.010	-0.007	180.104	0.001
0.019	0.030	0.031	0.031	0.001	113.269

BN-160

Density (g/cm^3): 2.01 | Space Group: 217
Bulk modulus (GPa): 163 | Shear modulus (GPa): 49
Young's modulus (GPa): 133 | Highest Young's modulus (GPa): 185
Hardness (GPa): 2 | Energy above hull (eV/atom): 0.30

Primitive Cell

1.000000

-3.95037128282076	3.95037128282076	3.95037128282076
3.95037128282076	-3.95037128282076	3.95037128282076
3.95037128282076	3.95037128282076	-3.95037128282076

B N

12 12

DIRECT

0.3931200349607664	0.3931200349607664	0.6167852528519182
0.6068799650392336	0.2236652178911518	0.0000000000000000
0.2236652178911518	0.6068799650392336	0.0000000000000000
0.7763347821088482	0.7763347821088482	0.3832147471480818
0.7763347821088482	0.3832147471480818	0.7763347821088482
0.6068799650392336	0.0000000000000000	0.2236652178911518
0.2236652178911518	0.0000000000000000	0.6068799650392336
0.3931200349607664	0.6167852528519182	0.3931200349607664
0.0000000000000000	0.2236652178911518	0.6068799650392336
0.3832147471480818	0.7763347821088482	0.7763347821088482
0.6167852528519182	0.3931200349607664	0.3931200349607664
0.0000000000000000	0.6068799650392336	0.2236652178911518
0.5855593930286430	0.5855593930286430	0.3601218655148052
0.4144406069713570	0.7745624724861622	-0.0000000000000001
0.7745624724861622	0.4144406069713569	-0.0000000000000001
0.2254375275138378	0.2254375275138378	0.6398781344851947
0.2254375275138378	0.6398781344851947	0.2254375275138378
0.4144406069713570	-0.0000000000000001	0.7745624724861622
0.7745624724861622	-0.0000000000000001	0.4144406069713570
0.5855593930286429	0.3601218655148051	0.5855593930286429
-0.0000000000000001	0.7745624724861622	0.4144406069713570
0.6398781344851948	0.2254375275138378	0.2254375275138378
0.3601218655148051	0.5855593930286429	0.5855593930286429
-0.0000000000000001	0.4144406069713569	0.7745624724861622

Stiffness tensor (GPa):

200.934	144.204	144.160	0.009	0.029	0.041
144.204	200.898	144.112	0.020	0.007	0.065
144.160	144.112	200.919	0.054	0.019	0.004
0.009	0.020	0.054	70.301	0.028	0.000
0.029	0.007	0.019	0.028	70.331	0.015
0.041	0.065	0.004	0.000	0.015	70.273

BN-161

Density (g/cm^3): 1.93 | Space Group: 44

Bulk modulus (GPa): 157 | Shear modulus (GPa): 90

Young's modulus (GPa): 226 | Highest Young's modulus (GPa): 693

Hardness (GPa): 11 | Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

-1.25490296709678	4.79690639245289	4.43872858309773
1.25490296709678	-4.79690639245289	4.43872858309773
1.25490296709678	4.79690639245289	-4.43872858309773

B N

5 5

DIRECT

0.7426167341467331	0.0507767044826031	0.6918400296641301
0.3589366748184730	0.0507767044826031	0.3081599703358699
0.0296194367983269	0.4024394936410716	0.6271799431572553
0.7752595504838162	0.4024394936410716	0.3728200568427447
0.6929985957596800	0.6929985957596800	0.0000000000000000
0.7677418832531075	0.9518421806568957	0.8158997025962118
0.1359424780606839	0.9518421806568957	0.1841002974037882
0.4644543549261776	0.5980353177368385	0.8664190371893392
0.7316162805474994	0.5980353177368385	0.1335809628106610
0.8008139913973353	0.3008139913973352	0.5000000000000000

Stiffness tensor (GPa):

716.315	82.226	54.120	0.041	0.023	0.008
82.226	290.162	187.558	-0.072	0.001	0.010
54.120	187.558	148.022	0.022	0.005	0.009
0.041	-0.072	0.022	143.735	0.016	0.065
0.023	0.001	0.005	0.016	121.547	0.010
0.008	0.010	0.009	0.065	0.010	164.890

BN-162

Density (g/cm^3): 1.81 | Space Group: 186
Bulk modulus (GPa): 171 | Shear modulus (GPa): 69
Young's modulus (GPa): 184 | Highest Young's modulus (GPa): 561
Hardness (GPa): 5 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

6.96102090722017	0.00000000000000	0.00000000000000
-3.48051045361009	6.02842094192727	0.00000000000000
0.00000000000000	0.00000000000000	4.33611267044643

B N

8 8

DIRECT

0.5497275318408290	0.0994550636816580	0.0875090604128822
0.9005449363183420	0.4502724681591710	0.0875090604128822
0.5497275318408290	0.4502724681591710	0.0875090604128822
0.4502724681591709	0.9005449363183420	0.5875090604128823
0.0994550636816580	0.5497275318408290	0.5875090604128823
0.4502724681591709	0.5497275318408290	0.5875090604128823
0.3333333333333333	0.6666666666666666	0.0591162336959122
0.6666666666666667	0.3333333333333333	0.5591162336959123
0.4510051128971359	0.9020102257942719	0.9157886250758043
0.0979897742057280	0.5489948871028640	0.9157886250758043
0.4510051128971359	0.5489948871028640	0.9157886250758043
0.5489948871028640	0.0979897742057281	0.4157886250758042
0.9020102257942719	0.4510051128971360	0.4157886250758042
0.5489948871028640	0.4510051128971360	0.4157886250758042
0.6666666666666667	0.3333333333333333	0.9309907122899087
0.3333333333333333	0.6666666666666666	0.4309907122899088

Stiffness tensor (GPa):

202.834	170.143	67.403	0.008	-0.017	-0.004
170.143	203.142	67.345	-0.016	-0.029	-0.021
67.403	67.345	584.919	0.014	0.008	-0.014
0.008	-0.016	0.014	138.159	0.004	0.009
-0.017	-0.029	0.008	0.004	138.198	-0.010
-0.004	-0.021	-0.014	0.009	-0.010	15.816

BN-163

Density (g/cm^3): 1.79
Space Group: 4
Bulk modulus (GPa): 93
Shear modulus (GPa): 56
Young's modulus (GPa): 141
Highest Young's modulus (GPa): 507
Hardness (GPa): 9
Energy above hull (eV/atom): 0.19

Primitive Cell

1.000000

7.33848448212511	0.00000000000000	0.00000000000000
0.00000000000000	4.41587660377650	0.00000000000000
-1.83561418454150	0.00000000000000	7.12360740165454

B N

10 10

DIRECT

0.7285054884186581	0.1088751835839609	0.9440170672013743
0.2714945115813418	0.6088751835839609	0.0559829327986257
0.0484152609366786	0.3990955693044065	0.2644479519992076
0.9515847390633214	0.8990955693044065	0.7355520480007924
0.0740984795115809	0.9258282811051490	0.0879565080123839
0.9259015204884191	0.4258282811051490	0.9120434919876161
0.9840793494455677	0.4057859340089753	0.5800118525481510
0.0159206505544323	0.9057859340089753	0.4199881474518490
0.4216936168523683	0.1003911853066841	0.0192917480206556
0.5783063831476316	0.6003911853066841	0.9807082519793444
0.2719559122890799	0.9275281602993921	0.0558699388272283
0.7280440877109200	0.4275281602993921	0.9441300611727717
0.9540443022243341	0.5751840138375980	0.7368163695557868
0.0459556977756659	0.0751840138375979	0.2631836304442132
0.9244865326768368	0.0552976807943262	0.9090249788825187
0.0755134673231632	0.5552976807943262	0.0909750211174813
0.0179034056752603	0.5730957883666570	0.4203698180527844
0.9820965943247397	0.0730957883666570	0.5796301819472156
0.5791776477861323	0.9289182040785022	0.9794720330899351
0.4208223522138676	0.4289182040785022	0.0205279669100649

Stiffness tensor (GPa):

294.850	93.989	134.299	-0.033	-74.767	0.014
93.989	547.731	75.416	0.007	-36.979	-0.020
134.299	75.416	164.292	-0.038	-71.598	-0.017
-0.033	0.007	-0.038	110.959	-0.013	-57.894
-74.767	-36.979	-71.598	-0.013	34.163	-0.005
0.014	-0.020	-0.017	-57.894	-0.005	151.823

BN-164

Density (g/cm^3): 1.73 | Space Group: 156
Bulk modulus (GPa): 90 | Shear modulus (GPa): 31
Young's modulus (GPa): 82 | Highest Young's modulus (GPa): 263
Hardness (GPa): 1 | Energy above hull (eV/atom): 0.56

Primitive Cell

1.000000

11.84790409519647	0.00000000000000	0.00000000000000
-5.92395204759823	10.26058592804182	0.00000000000000
0.00000000000000	0.00000000000000	3.52025869843730

B N

18 18

DIRECT

0.4058062951867450	0.5941937048132550	0.8102669198483829
0.0724735237672837	0.1449470475345674	0.1436177080920951
0.5217201947687713	0.2608600973843856	0.4769695731533561
0.2724387390545850	0.1362193695272925	0.2749241038203175
0.5304480448901916	0.4695519551098085	0.6082701052328939
0.1971141968295159	0.3942283936590317	0.9415722633094521
0.0724735237672837	0.9275264762327162	0.1436177080920951
0.7391399026156145	0.4782798052312287	0.4769695731533561
0.1883874096265098	0.5941937048132550	0.8102669198483829
0.9391039102196170	0.4695519551098085	0.6082701052328939
0.1971141968295158	0.8028858031704842	0.9415722633094521
0.8637806304727075	0.7275612609454150	0.2749241038203175
0.7391399026156145	0.2608600973843856	0.4769695731533561
0.4058062951867450	0.8116125903734901	0.8102669198483829
0.8550529524654326	0.9275264762327162	0.1436177080920951
0.6057716063409684	0.8028858031704842	0.9415722633094521
0.8637806304727075	0.1362193695272925	0.2749241038203175
0.5304480448901916	0.0608960897803830	0.6082701052328939
0.5962889717302886	0.4037110282697115	0.5112720041977886
0.9296215555935277	0.8592431111870553	0.1779155240266992
0.4740904407071538	0.7370452203535769	0.8445481928529858
0.7216542885300257	0.8608271442650128	0.0702061806854431
0.4725060799375113	0.5274939200624886	0.7368858112679839
0.8058387212029827	0.6116774424059654	0.4035515039821362
0.2629547796464231	0.7370452203535770	0.8445481928529858
0.5962889717302886	0.1925779434605770	0.5112720041977886
0.1407568888129447	0.0703784444064723	0.1779155240266992
0.3883225575940345	0.1941612787970173	0.4035515039821362
0.1391728557349871	0.8608271442650128	0.0702061806854431
0.4725060799375113	0.9450121598750227	0.7368858112679839
0.9296215555935277	0.0703784444064723	0.1779155240266992
0.2629547796464229	0.5259095592928461	0.8445481928529858
0.8074220565394230	0.4037110282697115	0.5112720041977886

0.0549878401249772	0.5274939200624886	0.7368858112679839
0.8058387212029827	0.1941612787970173	0.4035515039821362
0.1391728557349872	0.2783457114699743	0.0702061806854431

Stiffness tensor (GPa):

381.038	215.652	24.077	18.037	0.012	-0.028
215.652	381.178	24.379	-17.992	0.014	-0.035
24.077	24.379	32.667	-0.027	0.023	-0.056
18.037	-17.992	-0.027	6.916	0.004	0.005
0.012	0.014	0.023	0.004	6.985	17.875
-0.028	-0.035	-0.056	0.005	17.875	82.293

BN-165

Density (g/cm^3): 1.53 | Space Group: 38
Bulk modulus (GPa): 103 | Shear modulus (GPa): 61
Young's modulus (GPa): 152 | Highest Young's modulus (GPa): 553
Hardness (GPa): 9 | Energy above hull (eV/atom): 0.11

Primitive Cell

1.000000

2.51000594760304	0.00000000000000	0.00000000000000
0.00000000000000	6.52922924074288	5.75312406295102
0.00000000000000	-6.52922924074288	5.75312406295102

B N

7 7

DIRECT

0.5000000000000000	0.0128283277616331	0.2956464358924289
0.5000000000000000	0.2956464358924289	0.0128283277616331
0.5000000000000000	0.7902047979749141	0.9768658618393146
0.5000000000000000	0.9768658618393147	0.7902047979749141
0.0000000000000000	0.5423218086902836	0.9918515995769454
0.0000000000000000	0.9918515995769455	0.5423218086902835
0.0000000000000000	0.0452625166965967	0.0452625166965968
0.0000000000000000	0.9798504658670379	0.7094797626245357
0.0000000000000000	0.7094797626245357	0.9798504658670379
0.0000000000000000	0.2155899436661005	0.0188918370494255
0.0000000000000000	0.0188918370494255	0.2155899436661005
0.5000000000000000	0.4621883223208272	0.9978060444513739
0.5000000000000000	0.9978060444513739	0.4621883223208272
0.5000000000000000	0.9612122073015437	0.9612122073015438

Stiffness tensor (GPa):

574.109	68.852	44.848	-0.067	0.019	0.004
68.852	227.896	147.995	-0.089	0.009	-0.010
44.848	147.995	103.653	-0.081	0.011	-0.019
-0.067	-0.089	-0.081	105.610	0.005	-0.046
0.019	0.009	0.011	0.005	91.259	-0.000
0.004	-0.010	-0.019	-0.046	-0.000	133.582

BN-166

Density (g/cm^3): 1.32	Space Group: 217
Bulk modulus (GPa): 123	Shear modulus (GPa): 35
Young's modulus (GPa): 96	Highest Young's modulus (GPa): 229
Hardness (GPa): 1	Energy above hull (eV/atom): 0.75

Primitive Cell

1.000000

-3.96960356625557	3.96960356625557	3.96960356625557
3.96960356625557	-3.96960356625557	3.96960356625557
3.96960356625557	3.96960356625557	-3.96960356625557

B N

8 8

DIRECT

-0.0000000000000001	-0.0000000000000001	0.2005118500771591
0.0000000000000001	0.2005118500771592	-0.0000000000000000
0.2005118500771592	0.0000000000000001	-0.0000000000000000
0.7994881499228407	0.7994881499228407	0.7994881499228409
-0.0000000000000000	-0.0000000000000000	0.5882400391731343
0.0000000000000000	0.5882400391731344	0.0000000000000000
0.5882400391731344	0.0000000000000000	0.0000000000000000
0.4117599608268657	0.4117599608268657	0.4117599608268657
-0.0000000000000001	-0.0000000000000001	0.7913166643641103
0.0000000000000001	0.7913166643641104	0.0000000000000001
0.7913166643641104	0.0000000000000001	0.0000000000000001
0.2086833356358896	0.2086833356358896	0.2086833356358898
-0.0000000000000000	-0.0000000000000000	0.4045645822251265
0.0000000000000000	0.4045645822251265	-0.0000000000000000
0.4045645822251265	0.0000000000000000	0.0000000000000000
0.5954354177748735	0.5954354177748735	0.5954354177748735

Stiffness tensor (GPa):

128.737	119.926	119.914	0.007	-0.046	0.011
119.926	128.724	119.942	-0.013	0.003	-0.049
119.914	119.942	128.736	-0.057	0.000	0.001
0.007	-0.013	-0.057	96.394	-0.023	-0.020
-0.046	0.003	0.000	-0.023	96.384	-0.016
0.011	-0.049	0.001	-0.020	-0.016	96.389

BN-167

Density (g/cm^3): 1.29 | Space Group: 174

Bulk modulus (GPa): 127 | Shear modulus (GPa): 28

Young's modulus (GPa): 79 | Highest Young's modulus (GPa): 406

Hardness (GPa): -1 | Energy above hull (eV/atom): 0.30

Primitive Cell

1.000000

10.16299847917601	0.00000000000000	0.00000000000000
-5.08149923958801	8.80141486158904	0.00000000000000
0.00000000000000	0.00000000000000	2.50919754284796

B N

7 7

DIRECT

0.3333333333333333	0.6666666666666666	0.0000000000000000
0.0836066277694697	0.1672160600601384	0.0000000000000000
0.8327839399398616	0.9163905677093314	0.0000000000000000
0.0836094322906687	0.9163933722305303	0.0000000000000000
0.2083336258055231	0.4166650444434885	0.5000000000000000
0.5833349555565115	0.7916685813620346	0.5000000000000000
0.2083314186379654	0.7916663741944769	0.5000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.2488043999822038	0.4976037881045545	0.0000000000000000
0.5023962118954455	0.7512006118776493	0.0000000000000000
0.2487993881223507	0.7511956000177962	0.0000000000000000
0.1248835854484753	0.2497701188533811	0.5000000000000000
0.7502298811466188	0.8751134665950941	0.5000000000000000
0.1248865334049058	0.8751164145515247	0.5000000000000000

Stiffness tensor (GPa):

143.929	131.964	52.921	-0.067	-0.033	-0.009
131.964	143.389	53.390	0.125	-0.026	-0.029
52.921	53.390	426.665	-0.006	0.097	0.135
-0.067	0.125	-0.006	27.265	-0.011	0.022
-0.033	-0.026	0.097	-0.011	27.174	-0.124
-0.009	-0.029	0.135	0.022	-0.124	6.658

BN-168

Density (g/cm^3): 1.24
Space Group: 38
Bulk modulus (GPa): 87
Shear modulus (GPa): 40
Young's modulus (GPa): 104
Highest Young's modulus (GPa): 444
Hardness (GPa): 4
Energy above hull (eV/atom): 0.24

Primitive Cell

1.000000

2.52401596499655	0.00000000000000	0.00000000000000
0.00000000000000	4.79736279544441	10.98971196587289
0.00000000000000	-4.79736279544441	10.98971196587289

B N

8 8

DIRECT

0.0000000000000000	0.3323238060320512	0.3323238060320512
0.5000000000000000	0.6299285302764726	0.6299285302764726
0.5000000000000000	0.4327863638683280	0.4327863638683280
0.0000000000000000	0.8412563741650243	0.5816331493225717
0.0000000000000000	0.5816331493225717	0.8412563741650243
0.5000000000000000	0.0828935562619568	0.4591700012507953
0.5000000000000000	0.4591700012507953	0.0828935562619568
0.0000000000000000	0.5315695959852627	0.5315695959852627
0.0000000000000000	0.6674386555293830	0.6674386555293830
0.5000000000000000	0.3699334505532621	0.3699334505532621
0.5000000000000000	0.5670073645613518	0.5670073645613518
0.0000000000000000	0.1555827654189208	0.4216105320388228
0.0000000000000000	0.4216105320388228	0.1555827654189208
0.5000000000000000	0.9133501223533711	0.5452298856502995
0.5000000000000000	0.5452298856502995	0.9133501223533711
0.0000000000000000	0.4682857860252334	0.4682857860252334

Stiffness tensor (GPa):

463.504	34.610	60.186	0.038	0.015	0.007
34.610	69.747	102.515	0.052	-0.002	0.004
60.186	102.515	194.038	0.068	0.011	-0.019
0.038	0.052	0.068	2.577	-0.012	0.019
0.015	-0.002	0.011	-0.012	117.101	0.001
0.007	0.004	-0.019	0.019	0.001	60.450

BN-169

Density (g/cm^3): 0.87 | Space Group: 160

Bulk modulus (GPa): 70 | Shear modulus (GPa): 7

Young's modulus (GPa): 20 | Highest Young's modulus (GPa): 30

Hardness (GPa): -3 | Energy above hull (eV/atom): 1.29

Primitive Cell

1.000000

3.47268901656052	2.00495793852307	5.67086968159327
-3.47268901656052	2.00495793852307	5.67086968159327
0.00000000000000	-4.00991587704614	5.67086968159327

B N

5 5

DIRECT

0.2500001610626119	0.2500001610626119	0.2500001610626120
0.0880741704356490	0.0880741704356490	0.7357773918154296
0.0880742851920990	0.0880742851920990	0.0880742851920990
0.7357773918154294	0.0880741704356491	0.0880741704356491
0.0880741704356490	0.7357773918154296	0.0880741704356491
0.9999994616643019	0.9999994616643019	0.9999994616643021
0.1607837216932377	0.1607837216932377	0.5176490540173342
0.1607838587768492	0.1607838587768492	0.1607838587768493
0.5176490540173342	0.1607837216932377	0.1607837216932377
0.1607837216932377	0.5176490540173342	0.1607837216932377

Stiffness tensor (GPa):

75.063	67.385	67.383	0.288	0.415	0.405
67.385	75.044	67.378	0.424	0.286	0.412
67.383	67.378	75.046	0.428	0.422	0.271
0.288	0.424	0.428	10.510	-0.060	-0.074
0.415	0.286	0.422	-0.060	10.482	-0.070
0.405	0.412	0.271	-0.074	-0.070	10.486

BN-170

Density (g/cm^3): 0.84 | Space Group: 136
Bulk modulus (GPa): 61 | Shear modulus (GPa): 6
Young's modulus (GPa): 18 | Highest Young's modulus (GPa): 23
Hardness (GPa): -3 | Energy above hull (eV/atom): 1.30

Primitive Cell

1.000000

11.87194409969356	0.00000000000000	0.00000000000000
0.00000000000000	11.87194409969356	0.00000000000000
0.00000000000000	0.00000000000000	6.99741939890800

B N

20 20

DIRECT

0.6774862048717282	0.3225137951282718	0.4999999999999999
0.3225137951282718	0.6774862048717282	0.4999999999999999
0.1774862048717282	0.1774862048717281	0.0000000000000000
0.8225137951282718	0.8225137951282718	0.0000000000000000
0.6940806987456072	0.5534682752527693	0.4999999999999999
0.3059193012543928	0.4465317247472307	0.4999999999999999
0.4465317247472307	0.3059193012543928	0.4999999999999999
0.5534682752527693	0.6940806987456072	0.4999999999999999
0.0534682752527693	0.8059193012543928	0.0000000000000000
0.9465317247472307	0.1940806987456072	0.0000000000000000
0.8059193012543928	0.0534682752527693	0.0000000000000000
0.1940806987456072	0.9465317247472307	0.0000000000000000
0.7295744501481475	0.7295744501481475	0.6760391387640610
0.2704255498518525	0.2704255498518525	0.3239608612359390
0.2704255498518525	0.2704255498518525	0.6760391387640610
0.7295744501481475	0.7295744501481475	0.3239608612359390
0.2295744501481476	0.7704255498518525	0.1760391387640610
0.7704255498518525	0.2295744501481476	0.8239608612359389
0.7704255498518525	0.2295744501481476	0.1760391387640610
0.2295744501481476	0.7704255498518525	0.8239608612359389
0.6790077197272451	0.6790077197272451	0.4999999999999999
0.3209922802727549	0.3209922802727549	0.4999999999999999
0.1790077197272451	0.8209922802727549	0.0000000000000000
0.8209922802727549	0.1790077197272451	0.0000000000000000
0.5507623319614172	0.3035254564401511	0.4999999999999999
0.4492376680385828	0.6964745435598489	0.4999999999999999
0.3035254564401511	0.5507623319614172	0.4999999999999999
0.6964745435598489	0.4492376680385828	0.4999999999999999
0.1964745435598489	0.0507623319614172	0.0000000000000000
0.8035254564401511	0.9492376680385828	0.0000000000000000
0.9492376680385828	0.8035254564401511	0.0000000000000000
0.0507623319614172	0.1964745435598489	0.0000000000000000
0.7292235899676489	0.2707764100323511	0.6774518022107119

0.2707764100323511	0.7292235899676489	0.3225481977892881
0.2707764100323511	0.7292235899676489	0.6774518022107119
0.7292235899676489	0.2707764100323511	0.3225481977892881
0.2292235899676489	0.2292235899676489	0.1774518022107121
0.7707764100323511	0.7707764100323511	0.8225481977892880
0.7707764100323511	0.7707764100323511	0.1774518022107121
0.2292235899676489	0.2292235899676489	0.8225481977892880

Stiffness tensor (GPa):

63.418	54.072	62.904	-0.068	0.004	0.042
54.072	63.716	62.658	0.006	-0.006	-0.030
62.904	62.658	90.281	-0.074	-0.002	-0.016
-0.068	0.006	-0.074	5.616	0.002	0.002
0.004	-0.006	-0.002	0.002	5.670	-0.006
0.042	-0.030	-0.016	0.002	-0.006	6.990

BN-171

Density (g/cm^3): 0.75 | Space Group: 217

Bulk modulus (GPa): 69 | Shear modulus (GPa): 17

Young's modulus (GPa): 48 | Highest Young's modulus (GPa): 130

Hardness (GPa): -1 | Energy above hull (eV/atom): 0.82

Primitive Cell

1.000000

-5.48692355182117	5.48692355182117	5.48692355182117
5.48692355182117	-5.48692355182117	5.48692355182117
5.48692355182117	5.48692355182117	-5.48692355182117

B N

12 12

DIRECT

-0.0000000000000000	-0.0000000000000000	0.8530716005646783
0.0000000000000000	0.8530716005646783	-0.0000000000000000
0.8530716005646783	0.0000000000000000	-0.0000000000000000
0.1469283994353217	0.1469283994353217	0.1469283994353217
-0.0000000000000001	-0.0000000000000001	0.5725356512307609
0.0000000000000001	0.5725356512307610	-0.0000000000000001
0.5725356512307610	0.0000000000000001	-0.0000000000000001
0.4274643487692390	0.4274643487692390	0.4274643487692391
0.0000000000000000	0.0000000000000000	0.2967941271131873
0.0000000000000000	0.2967941271131873	0.0000000000000000
0.2967941271131873	0.0000000000000000	0.0000000000000000
0.7032058728868127	0.7032058728868127	0.7032058728868127
-0.0000000000000001	-0.0000000000000001	0.1512932791256778
0.0000000000000001	0.1512932791256779	-0.0000000000000001
0.1512932791256779	0.0000000000000001	-0.0000000000000001
0.8487067208743221	0.8487067208743221	0.8487067208743222
-0.0000000000000001	-0.0000000000000001	0.4308006567570677
0.0000000000000001	0.4308006567570678	-0.0000000000000000
0.4308006567570678	0.0000000000000001	-0.0000000000000000
0.5691993432429322	0.5691993432429322	0.5691993432429323
0.0000000000000000	0.0000000000000000	0.7069235564868710
0.0000000000000000	0.7069235564868710	0.0000000000000000
0.7069235564868710	0.0000000000000000	0.0000000000000000
0.2930764435131290	0.2930764435131290	0.2930764435131290

Stiffness tensor (GPa):

69.791	68.401	68.407	-0.040	0.002	0.010
68.401	69.781	68.406	0.006	-0.052	-0.005
68.407	68.406	69.774	0.001	0.003	-0.056
-0.040	0.006	0.001	54.855	-0.016	-0.020
0.002	-0.052	0.003	-0.016	54.827	0.024
0.010	-0.005	-0.056	-0.020	0.024	54.828

BN-172

Density (g/cm^3): 3.88
Space Group: 215
Bulk modulus (GPa): 392
Shear modulus (GPa): 332
Young's modulus (GPa): 776
Highest Young's modulus (GPa): 1236
Hardness (GPa): 46
Energy above hull (eV/atom): 1.76

Primitive Cell

1.000000

3.49021633217034	0.00000000000000	0.00000000000000
0.00000000000000	3.49021633217034	0.00000000000000
0.00000000000000	0.00000000000000	3.49021633217034

B N

4 4

DIRECT

0.7501217175029078	0.7501217175029078	0.2498782824970921
0.2498782824970922	0.2498782824970922	0.2498782824970921
0.2498782824970922	0.7501217175029078	0.7501217175029079
0.7501217175029078	0.2498782824970922	0.7501217175029079
0.2499373551885134	0.2499373551885134	0.7500626448114865
0.7500626448114867	0.7500626448114867	0.7500626448114865
0.7500626448114867	0.2499373551885134	0.2499373551885134
0.2499373551885134	0.7500626448114867	0.2499373551885134

Stiffness tensor (GPa):

552.506	311.271	311.272	-0.046	-0.052	-0.077
311.271	552.422	311.216	-0.052	-0.046	-0.078
311.272	311.216	552.415	-0.053	-0.052	-0.086
-0.046	-0.052	-0.053	634.601	-0.001	-0.002
-0.052	-0.046	-0.052	-0.001	634.600	0.001
-0.077	-0.078	-0.086	-0.002	0.001	634.633

BN-173

Density (g/cm^3): 3.41 | Space Group: 10
Bulk modulus (GPa): 363 | Shear modulus (GPa): 351
Young's modulus (GPa): 797 | Highest Young's modulus (GPa): 933
Hardness (GPa): 56 | Energy above hull (eV/atom): 0.10

Primitive Cell

1.000000

4.28673600876502	0.00000000000000	0.00000000000000
0.00000000000000	2.54867132077904	0.00000000000000
-0.00523917403480	0.00000000000000	17.71504087808720

B N

16 16

DIRECT

0.1707512531132681	0.5000000000000000	0.3305061056643607
0.8292487468867319	0.5000000000000000	0.6694938943356392
0.1725498833115587	0.5000000000000000	0.0831670758380241
0.8274501166884413	0.5000000000000000	0.9168329241619759
0.6737062246731906	0.5000000000000000	0.1666282395431018
0.3262937753268094	0.5000000000000000	0.8333717604568982
0.8285169717026649	0.5000000000000000	0.4190909770776456
0.1714830282973351	0.5000000000000000	0.5809090229223544
0.3300661742787517	0.0000000000000000	0.4554397672465737
0.6699338257212483	0.0000000000000000	0.5445602327534262
0.1735932737894602	0.0000000000000000	0.2080596771895671
0.8264067262105398	0.0000000000000000	0.7919403228104329
0.6718407567163812	0.0000000000000000	0.0441133465604200
0.3281592432836188	0.0000000000000000	0.9558866534395800
0.6732464413681363	0.0000000000000000	0.2914655376834959
0.3267535586318637	0.0000000000000000	0.7085344623165042
0.1962862639987414	0.5000000000000000	0.4197434543432649
0.8037137360012586	0.5000000000000000	0.5802565456567350
0.2985923551180411	0.5000000000000000	0.1668990458178809
0.7014076448819589	0.5000000000000000	0.8331009541821190
0.8010720746653028	0.5000000000000000	0.0830518463703651
0.1989279253346972	0.5000000000000000	0.9169481536296349
0.8013249759345774	0.5000000000000000	0.3300847644318234
0.1986750240654226	0.5000000000000000	0.6699152355681766
0.3014389239760068	0.0000000000000000	0.2918358919107286
0.6985610760239932	0.0000000000000000	0.7081641080892713
0.3003466137877856	0.0000000000000000	0.0443133043137907
0.6996533862122144	0.0000000000000000	0.9556866956862093
0.7985984543493276	0.0000000000000000	0.2077452467429057
0.2014015456506724	0.0000000000000000	0.7922547532570943
0.6959038933561319	0.0000000000000000	0.4548828799932004
0.3040961066438681	0.0000000000000000	0.5451171200067997

Stiffness tensor (GPa):

854.842	76.035	100.181	0.009	1.547	0.015
76.035	956.830	128.658	0.013	0.084	0.040
100.181	128.658	855.125	-0.002	-1.359	0.054
0.009	0.013	-0.002	374.059	0.007	-0.018
1.547	0.084	-1.359	0.007	276.509	0.002
0.015	0.040	0.054	-0.018	0.002	334.920

BN-174

Density (g/cm^3): 3.38 | Space Group: 10
Bulk modulus (GPa): 359 | Shear modulus (GPa): 340
Young's modulus (GPa): 775 | Highest Young's modulus (GPa): 935
Hardness (GPa): 54 | Energy above hull (eV/atom): 0.11

Primitive Cell

1.000000

4.31687501829202	0.00000000000000	0.00000000000000
0.00000000000000	2.54822740463638	0.00000000000000
-0.00401706891031	0.00000000000000	13.29332705437629

B N

12 12

DIRECT

0.6728242620231123	0.0000000000000000	0.5586139589439345
0.3271757379768877	0.0000000000000000	0.4413860410560654
0.8279907793888620	0.0000000000000000	0.8922097374993454
0.1720092206111380	0.0000000000000000	0.1077902625006546
0.1716432149731784	0.0000000000000000	0.7745255308542845
0.8283567850268216	0.0000000000000000	0.2254744691457154
0.3294579732605964	0.5000000000000000	0.9408576369598115
0.6705420267394036	0.5000000000000000	0.0591423630401885
0.1737527201560126	0.5000000000000000	0.6107822457648062
0.8262472798439874	0.5000000000000000	0.3892177542351937
0.6743164275986331	0.5000000000000000	0.7224362837934508
0.3256835724013669	0.5000000000000000	0.2775637162065492
0.8027964637134740	0.0000000000000000	0.7735226945368031
0.1972035362865260	0.0000000000000000	0.2264773054631969
0.1947030902100325	0.0000000000000000	0.8935854877619660
0.8052969097899675	0.0000000000000000	0.1064145122380340
0.3019676750734214	0.0000000000000000	0.5594348730160728
0.6980323249265786	0.0000000000000000	0.4405651269839272
0.3024727248221682	0.5000000000000000	0.7232529683210900
0.6975272751778318	0.5000000000000000	0.2767470316789101
0.8022420564996265	0.5000000000000000	0.6101556668218513
0.1977579435003735	0.5000000000000000	0.3898443331781486
0.6943024584059021	0.5000000000000000	0.9395765977673317
0.3056975415940979	0.5000000000000000	0.0604234022326683

Stiffness tensor (GPa):

807.548	81.947	114.116	0.011	1.287	0.009
81.947	959.867	125.645	0.014	-0.053	0.039
114.116	125.645	824.959	0.003	-1.304	0.047
0.011	0.014	0.003	363.588	0.007	-0.045
1.287	-0.053	-1.304	0.007	262.797	-0.000
0.009	0.039	0.047	-0.045	-0.000	334.746

BN-175

Density (g/cm^3): 3.38 | Space Group: 45
Bulk modulus (GPa): 357 | Shear modulus (GPa): 353
Young's modulus (GPa): 796 | Highest Young's modulus (GPa): 1005
Hardness (GPa): 58 | Energy above hull (eV/atom): 0.14

Primitive Cell

1.000000

-2.25080509070152	7.71897575646125	2.10635883496367
2.25080509070152	-7.71897575646125	2.10635883496367
2.25080509070152	7.71897575646125	-2.10635883496367

B N

12 12

DIRECT

0.2432106373149872	0.3540022292748385	0.2053503467112244
0.1486518825636141	0.0378602906037627	0.7946496532887755
0.6486518825636141	0.8540022292748386	0.1107915919598514
0.7432106373149872	0.5378602906037627	0.8892084080401488
0.4037858854018741	0.3594318523045806	0.3733636950306001
0.9860681572739805	0.0304221903712740	0.6266363049693999
0.4860681572739805	0.8594318523045805	0.9556459669027064
0.9037858854018741	0.5304221903712739	0.0443540330972935
0.8224712041404596	0.0368940705856558	0.4672729061256569
0.5696211644599989	0.3551982980148027	0.5327270938743431
0.0696211644599989	0.5368940705856557	0.2144228664451961
0.3224712041404596	0.8551982980148027	0.7855771335548039
0.6151948769499662	0.7440273629802470	0.2252640652549294
0.5187632977253175	0.3899308116950368	0.7747359347450706
0.0187632977253175	0.2440273629802469	0.1288324860302807
0.1151948769499662	0.8899308116950368	0.8711675139697194
0.1945531741831509	0.4014643557477884	0.4590217586164909
0.9424425971312975	0.7355314155666601	0.5409782413835091
0.4424425971312975	0.9014643557477884	0.2069111815646374
0.6945531741831509	0.2355314155666600	0.7930888184353626
0.7787245536370981	0.7378468147635473	0.3773345645023426
0.3605122502612048	0.4013899891347554	0.6226654354976573
0.8605122502612048	0.2378468147635474	0.9591222611264494
0.2787245536370981	0.9013899891347554	0.0408777388735507

Stiffness tensor (GPa):

770.072	172.654	46.371	0.016	0.037	0.008
172.654	877.893	63.557	0.012	0.019	0.035
46.371	63.557	1010.683	0.004	0.010	0.037
0.016	0.012	0.004	334.390	0.007	-0.006
0.037	0.019	0.010	0.007	297.320	0.004
0.008	0.035	0.037	-0.006	0.004	362.522

BN-176

Density (g/cm^3): 3.36 | Space Group: 10

Bulk modulus (GPa): 346 | Shear modulus (GPa): 336

Young's modulus (GPa): 762 | Highest Young's modulus (GPa): 872

Hardness (GPa): 55 | Energy above hull (eV/atom): 0.37

Primitive Cell

1.000000

10.11843415973446	0.00000000000000	0.00000000000000
0.00000000000000	2.55480046941572	0.00000000000000
-1.97869129993312	0.00000000000000	13.28213120694981

B N

28 28

DIRECT

0.7488192785543081	0.0000000000000000	0.8225624395563806
0.2511807214456919	0.0000000000000000	0.1774375604436193
0.9884016788374357	0.0000000000000000	0.8871745518454612
0.0115983211625643	0.0000000000000000	0.1128254481545388
0.5121702419201228	0.0000000000000000	0.1234611550936618
0.4878297580798772	0.0000000000000000	0.8765388449063382
0.9666359891148094	0.0000000000000000	0.7595020122183930
0.0333640108851906	0.0000000000000000	0.2404979877816070
0.9019539158810349	0.0000000000000000	0.5292661135683183
0.0980460841189651	0.0000000000000000	0.4707338864316816
0.7632711422208487	0.5000000000000000	0.6537989387516523
0.2367288577791513	0.5000000000000000	0.3462010612483477
0.1725630557078968	0.5000000000000000	0.0158118423342249
0.8274369442921032	0.5000000000000000	0.9841881576657751
0.3317241236369816	0.5000000000000000	0.9857251568469694
0.6682758763630184	0.5000000000000000	0.0142748431530306
0.1526884566012374	0.5000000000000000	0.8284400501608362
0.8473115433987626	0.5000000000000000	0.1715599498391638
0.1022028457337952	0.5000000000000000	0.6364897776977672
0.8977971542662048	0.5000000000000000	0.3635102223022328
0.6882077013470802	0.5000000000000000	0.4545436484111383
0.3117922986529198	0.5000000000000000	0.5454563515888617
0.4582851676153401	0.5000000000000000	0.2662738418009457
0.5417148323846599	0.5000000000000000	0.7337261581990544
0.4479047883984191	0.0000000000000000	0.4263510093617717
0.5520952116015809	0.0000000000000000	0.5736489906382283
0.3093797802103740	0.0000000000000000	0.7192425391245314
0.6906202197896260	0.0000000000000000	0.2807574608754685
0.4625575568476062	0.0000000000000000	0.7576611560094121
0.5374424431523938	0.0000000000000000	0.2423388439905879
0.8086854314874804	0.0000000000000000	0.7172207289349761
0.1913145685125196	0.0000000000000000	0.2827792710650238
0.1529735735178051	0.0000000000000000	0.0797887650518916

0.8470264264821949	0.0000000000000000	0.9202112349481084
0.3562263373890969	0.0000000000000000	0.9196070997539776
0.6437736626109031	0.0000000000000000	0.0803929002460224
0.2446089578385711	0.0000000000000000	0.8246341632067407
0.7553910421614289	0.0000000000000000	0.1753658367932593
0.6041029972291307	0.0000000000000000	0.4682102177577529
0.3958970027708693	0.0000000000000000	0.5317897822422470
0.6587308714142202	0.5000000000000000	0.8208098137600059
0.3412691285857798	0.5000000000000000	0.1791901862399940
0.0749081178102200	0.5000000000000000	0.9171534609009213
0.9250918821897800	0.5000000000000000	0.0828465390990787
0.4248859812754369	0.5000000000000000	0.0920048308622164
0.5751140187245631	0.5000000000000000	0.9079951691377836
0.0452490454840792	0.5000000000000000	0.7340760681701823
0.9547509545159208	0.5000000000000000	0.2659239318298176
0.2631031313320263	0.5000000000000000	0.6557836246484099
0.7368968686679737	0.5000000000000000	0.3442163753515901
0.8163808429890476	0.5000000000000000	0.5459394208179649
0.1836191570109524	0.5000000000000000	0.4540605791820351
0.4009890767474426	0.5000000000000000	0.3664789707393385
0.5990109232525574	0.5000000000000000	0.6335210292606615
0.0560325173276172	0.0000000000000000	0.5778333310262300
0.9439674826723828	0.0000000000000000	0.4221666689737699

Stiffness tensor (GPa):

779.656	97.343	159.913	0.012	7.346	0.024
97.343	888.598	78.252	0.004	7.399	0.037
159.913	78.252	775.070	0.006	-16.628	0.017
0.012	0.004	0.006	318.990	0.002	5.011
7.346	7.399	-16.628	0.002	344.209	0.013
0.024	0.037	0.017	5.011	0.013	322.870

BN-177

Density (g/cm^3): 3.34 | Space Group: 12

Bulk modulus (GPa): 341 | Shear modulus (GPa): 311

Young's modulus (GPa): 715 | Highest Young's modulus (GPa): 873

Hardness (GPa): 49 | Energy above hull (eV/atom): 0.18

Primitive Cell

1.000000

6.64500285102175	-1.28208892424570	0.00000000000000
6.64500285102175	1.28208892424570	0.00000000000000
-0.05841485309351	0.00000000000000	4.34674671013368

B N

6 6

DIRECT

0.0581667865215605	0.0581667865215605	0.3292154768533995
0.9418332134784395	0.9418332134784395	0.6707845231466005
0.2810104606512322	0.2810104606512323	0.6712711634902699
0.7189895393487677	0.7189895393487677	0.3287288365097300
0.6112771909784609	0.6112771909784609	0.8314657078163968
0.3887228090215391	0.3887228090215391	0.1685342921836031
0.2806923844752229	0.2806923844752229	0.2934934945923213
0.7193076155247771	0.7193076155247771	0.7065065054076787
0.0593057228773447	0.0593057228773447	0.6997763614908221
0.9406942771226552	0.9406942771226553	0.3002236385091778
0.6097856098556020	0.6097856098556020	0.1988270461835419
0.3902143901443979	0.3902143901443980	0.8011729538164581

Stiffness tensor (GPa):

871.641	134.855	98.374	0.026	-13.055	-0.020
134.855	898.782	71.757	0.031	-11.254	0.008
98.374	71.757	709.473	0.025	3.060	0.012
0.026	0.031	0.025	254.443	-0.003	-9.011
-13.055	-11.254	3.060	-0.003	237.333	0.002
-0.020	0.008	0.012	-9.011	0.002	368.856

BN-178

Density (g/cm^3): 3.29 | Space Group: 8
Bulk modulus (GPa): 330 | Shear modulus (GPa): 328
Young's modulus (GPa): 739 | Highest Young's modulus (GPa): 879
Hardness (GPa): 56 | Energy above hull (eV/atom): 0.54

Primitive Cell

1.000000

4.59190642459125	-1.27805890880229	0.00000000000000
4.59190642459125	1.27805890880229	0.00000000000000
-0.49884741772633	0.00000000000000	4.26652464066340

B N

4 4

DIRECT

0.8933548175770432	0.8933548175770432	0.7429763434118187
0.2258511425404489	0.2258511425404490	0.0559964858432674
0.1563893339960609	0.1563893339960609	0.6799571496098139
0.5080671438914867	0.5080671438914868	0.2730523910571142
0.3985779221534598	0.3985779221534598	0.9663689080796671
0.0010009152120036	0.0010009152120036	0.4875648016704026
0.7316496256724365	0.7316496256724366	0.5688155459026325
0.6853091557192805	0.6853091557192807	0.2252684114252767

Stiffness tensor (GPa):

662.812	75.340	130.919	0.029	21.183	-0.012
75.340	863.217	96.341	0.019	-33.580	-0.022
130.919	96.341	865.550	0.013	45.295	-0.030
0.029	0.019	0.013	386.648	0.006	-21.545
21.183	-33.580	45.295	0.006	328.962	-0.002
-0.012	-0.022	-0.030	-21.545	-0.002	255.800

BN-179

Density (g/cm^3): 3.27 | Space Group: 36
Bulk modulus (GPa): 312 | Shear modulus (GPa): 289
Young's modulus (GPa): 663 | Highest Young's modulus (GPa): 831
Hardness (GPa): 47 | Energy above hull (eV/atom): 0.22

Primitive Cell

1.000000

1.29042745511671	-6.61828084154798	0.00000000000000
1.29042745511671	6.61828084154798	0.00000000000000
0.00000000000000	0.00000000000000	4.42798405894729

B N

6 6

DIRECT

0.7213201272815177	0.2786798727184824	0.0899418672019456
0.2786798727184823	0.7213201272815177	0.5899418672019456
0.6148781597794453	0.3851218402205547	0.5907098296071995
0.3851218402205547	0.6148781597794453	0.0907098296071995
0.9481445335100160	0.0518554664899840	0.7581123289215616
0.0518554664899840	0.9481445335100160	0.2581123289215616
0.7227833569693403	0.2772166430306597	0.7180750808920255
0.2772166430306597	0.7227833569693403	0.2180750808920253
0.0523982520013644	0.9476017479986356	0.6240191610854966
0.9476017479986356	0.0523982520013644	0.1240191610854966
0.3855031131618600	0.6144968868381400	0.7201416593115073
0.6144968868381400	0.3855031131618600	0.2201416593115071

Stiffness tensor (GPa):

836.918	139.528	72.767	0.019	0.016	-0.002
139.528	877.739	121.065	-0.096	0.008	-0.020
72.767	121.065	520.500	-0.065	0.008	-0.018
0.019	-0.096	-0.065	294.344	0.020	0.012
0.016	0.008	0.008	0.020	201.710	0.004
-0.002	-0.020	-0.018	0.012	0.004	358.585

BN-180

Density (g/cm^3): 3.21 | Space Group: 27

Bulk modulus (GPa): 330 | Shear modulus (GPa): 298

Young's modulus (GPa): 687 | Highest Young's modulus (GPa): 968

Hardness (GPa): 47 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.73267321189906	0.00000000000000	0.00000000000000
0.00000000000000	12.86231723680054	0.00000000000000
0.00000000000000	0.00000000000000	4.21541463516937

B N

20 20

DIRECT

0.3442426144112738	0.5564117078487254	0.6677598715698785
0.6557573855887262	0.4435882921512746	0.6677598715698785
0.3442426144112738	0.4435882921512746	0.1677598715698785
0.6557573855887262	0.5564117078487254	0.1677598715698785
0.1543219304267405	0.6499846036032875	0.1674057381200680
0.8456780695732595	0.3500153963967125	0.1674057381200680
0.1543219304267405	0.3500153963967125	0.6674057381200680
0.8456780695732595	0.6499846036032875	0.6674057381200680
0.8530273020365736	0.9426633775425568	0.1670435756036506
0.1469726979634264	0.0573366224574432	0.1670435756036506
0.8530273020365736	0.0573366224574432	0.6670435756036506
0.1469726979634264	0.9426633775425568	0.6670435756036506
0.6485273720297349	0.8567890453751525	0.6676890170848176
0.3514726279702651	0.1432109546248475	0.6676890170848176
0.6485273720297349	0.1432109546248475	0.1676890170848178
0.3514726279702651	0.8567890453751525	0.1676890170848178
0.3461024381611950	0.7432020533271764	0.6676479922607272
0.6538975618388050	0.2567979466728236	0.6676479922607272
0.3461024381611950	0.2567979466728236	0.1676479922607272
0.6538975618388050	0.7432020533271764	0.1676479922607272
0.3251847644077421	0.5568791526070347	0.2967345025779611
0.6748152355922579	0.4431208473929653	0.2967345025779611
0.3251847644077421	0.4431208473929653	0.7967345025779611
0.6748152355922579	0.5568791526070347	0.7967345025779611
0.1639313786166223	0.6503271503057204	0.7962968291611590
0.8360686213833777	0.3496728496942796	0.7962968291611590
0.1639313786166223	0.3496728496942796	0.2962968291611590
0.8360686213833777	0.6503271503057204	0.2962968291611590
0.8335420841486159	0.9407361922253679	0.7988850845742095
0.1664579158513841	0.0592638077746321	0.7988850845742095
0.8335420841486159	0.0592638077746321	0.2988850845742095
0.1664579158513841	0.9407361922253679	0.2988850845742095
0.6675540515617653	0.8588262841788366	0.2988983071484227

0.3324459484382347	0.1411737158211634	0.2988983071484227
0.6675540515617653	0.1411737158211634	0.7988983071484227
0.3324459484382347	0.8588262841788366	0.7988983071484227
0.3281446385158517	0.7421117721235482	0.2966391309155441
0.6718553614841483	0.2578882278764518	0.2966391309155441
0.3281446385158517	0.2578882278764518	0.7966391309155441
0.6718553614841483	0.7421117721235482	0.7966391309155441

Stiffness tensor (GPa):

569.589	241.272	41.983	0.015	0.020	0.005
241.272	754.612	67.229	0.011	0.006	0.019
41.983	67.229	975.032	0.001	0.013	0.016
0.015	0.011	0.001	320.514	0.006	0.012
0.020	0.006	0.013	0.006	262.676	0.011
0.005	0.019	0.016	0.012	0.011	305.285

BN-181

Density (g/cm^3): 3.21	Space Group: 8
Bulk modulus (GPa): 296	Shear modulus (GPa): 237
Young's modulus (GPa): 561	Highest Young's modulus (GPa): 950
Hardness (GPa): 35	Energy above hull (eV/atom): 0.31

Primitive Cell

1.000000

4.12318443573982	-1.31732131184864	0.00000000000000
4.12318443573982	1.31732131184864	0.00000000000000
-3.78387739836478	0.00000000000000	4.72927291282000

B N

4 4

DIRECT

0.2664484392674096	0.2664484392674096	0.2722165066839773
0.5177295346876367	0.5177295346876367	0.8136469712842228
0.6624011874097973	0.6624011874097973	0.5309673514258905
0.8911998462018492	0.8911998462018492	0.0542323565164585
0.6804336518034253	0.6804336518034253	0.7851976857710444
0.4348598097140353	0.4348598097140353	0.2500160073141729
0.2882006461085593	0.2882006461085593	0.5326955749626743
0.0513268617479783	0.0513268617479783	0.0036274960415580

Stiffness tensor (GPa):

936.513	80.035	156.084	0.020	-8.639	-0.007
80.035	400.528	94.353	-0.073	-29.700	-0.005
156.084	94.353	895.337	0.009	41.949	0.002
0.020	-0.073	0.009	143.452	-0.013	-8.722
-8.639	-29.700	41.949	-0.013	397.801	0.001
-0.007	-0.005	0.002	-8.722	0.001	144.460

BN-182

Density (g/cm^3): 2.99 | Space Group: 108
Bulk modulus (GPa): 243 | Shear modulus (GPa): 207
Young's modulus (GPa): 484 | Highest Young's modulus (GPa): 856
Hardness (GPa): 35 | Energy above hull (eV/atom): 0.35

Primitive Cell

1.000000

-4.43006445536250	4.43006445536250	2.10488042828588
4.43006445536250	-4.43006445536250	2.10488042828588
4.43006445536250	4.43006445536250	-2.10488042828588

B N

12 12

DIRECT

0.9998902658877196	0.1270357065231189	0.2912450671321384
0.8357906393909804	0.7086451987555813	0.7087549328678616
0.1270357065231190	0.8357906393909804	0.1271454406353993
0.7086451987555812	0.9998902658877196	0.8728545593646007
0.3357906393909805	0.6270357065231189	0.1271454406353993
0.4998902658877196	0.2086451987555812	0.8728545593646008
0.2086451987555812	0.3357906393909805	0.7087549328678615
0.6270357065231189	0.4998902658877196	0.2912450671321385
0.5519524179742938	0.7318369269342654	0.5000000000000000
0.2318369269342654	0.0519524179742938	0.5000000000000000
0.7318369269342655	0.2318369269342654	0.1798845089599716
0.0519524179742938	0.5519524179742938	0.8201154910400283
0.6285050515824391	0.7473983027873292	0.2856037660163247
0.4617945367710044	0.3429012855661144	0.7143962339836752
0.7473983027873292	0.4617945367710045	0.1188932512048901
0.3429012855661144	0.6285050515824391	0.8811067487951099
0.9617945367710043	0.2473983027873292	0.1188932512048900
0.1285050515824391	0.8429012855661144	0.8811067487951099
0.8429012855661144	0.9617945367710045	0.7143962339836754
0.2473983027873292	0.1285050515824390	0.2856037660163246
0.2060261751114975	0.4142234758580591	0.5000000000000000
0.9142234758580592	0.7060261751114976	0.5000000000000000
0.4142234758580591	0.9142234758580592	0.2081973007465616
0.7060261751114976	0.2060261751114975	0.7918026992534384

Stiffness tensor (GPa):

416.259	198.930	31.997	0.037	-0.024	0.007
198.930	416.870	31.962	-0.092	-0.020	0.004
31.997	31.962	859.775	-0.019	-0.020	0.005
0.037	-0.092	-0.019	240.559	0.003	0.015
-0.024	-0.020	-0.020	0.003	240.557	0.016
0.007	0.004	0.005	0.015	0.016	165.938

BN-183

Density (g/cm^3): 2.86 | Space Group: 39
Bulk modulus (GPa): 294 | Shear modulus (GPa): 197
Young's modulus (GPa): 483 | Highest Young's modulus (GPa): 882
Hardness (GPa): 24 | Energy above hull (eV/atom): 0.21

Primitive Cell

1.000000

9.61638601838598	0.00000000000000	0.00000000000000
0.00000000000000	3.52470241135900	2.12435396851702
0.00000000000000	-3.52470241135900	2.12435396851702

B N

10 10

DIRECT

0.6825958711099868	0.4381920012547844	0.2294554344475366
0.3174041288900132	0.2294554344475366	0.4381920012547844
0.6825958711099868	0.7294554344475366	0.9381920012547844
0.3174041288900132	0.9381920012547844	0.7294554344475366
0.5772000977664024	0.0827249855685219	0.5827249855685219
0.4227999022335976	0.5827249855685219	0.0827249855685219
0.0622438669085228	0.1035571267300562	0.6035571267300561
0.9377561330914772	0.6035571267300561	0.1035571267300562
0.2067815913646833	0.5824044353193687	0.0824044353193687
0.7932184086353167	0.0824044353193687	0.5824044353193687
0.6830755645611196	0.7944216900734147	0.6076459258064735
0.3169244354388804	0.6076459258064735	0.7944216900734147
0.6830755645611196	0.1076459258064735	0.2944216900734147
0.3169244354388804	0.2944216900734147	0.1076459258064735
0.5688692321480834	0.4515161704394905	0.9515161704394905
0.4311307678519166	0.9515161704394905	0.4515161704394905
0.0661992896054882	0.4365667234252102	0.9365667234252102
0.9338007103945118	0.9365667234252102	0.4365667234252102
0.1995995191656492	0.9491783940306113	0.4491783940306113
0.8004004808343508	0.4491783940306113	0.9491783940306113

Stiffness tensor (GPa):

808.297	62.622	98.335	0.043	0.032	0.079
62.622	584.643	44.220	0.028	-0.014	-0.037
98.335	44.220	895.819	0.004	0.014	0.117
0.043	0.028	0.004	204.006	0.001	0.004
0.032	-0.014	0.014	0.001	298.464	-0.010
0.079	-0.037	0.117	0.004	-0.010	48.972

BN-184

Density (g/cm^3): 2.79 | Space Group: 65

Bulk modulus (GPa): 253 | Shear modulus (GPa): 153

Young's modulus (GPa): 382 | Highest Young's modulus (GPa): 896

Hardness (GPa): 18 | Energy above hull (eV/atom): 0.15

Primitive Cell

1.000000

3.11778367834744	-7.50657723228373	0.00000000000000
3.11778367834744	7.50657723228373	0.00000000000000
0.00000000000000	0.00000000000000	2.52738590905239

B N

8 8

DIRECT

0.8669064480084288	0.1330935519915713	0.0000000000000000
0.1330935519915714	0.8669064480084288	0.0000000000000000
0.1782796203838141	0.1782796203838142	0.5000000000000000
0.8217203796161858	0.8217203796161858	0.5000000000000000
0.4237029746740040	0.5762970253259960	0.0000000000000000
0.5762970253259960	0.4237029746740040	0.0000000000000000
0.2768003952617699	0.7231996047382301	0.5000000000000000
0.7231996047382301	0.2768003952617700	0.5000000000000000
0.9193219119276702	0.0806780880723298	0.5000000000000000
0.0806780880723298	0.9193219119276702	0.5000000000000000
0.3103821798669017	0.3103821798669018	0.0000000000000000
0.6896178201330982	0.6896178201330982	0.0000000000000000
0.2266646927087638	0.7733353072912362	0.0000000000000000
0.7733353072912362	0.2266646927087638	0.0000000000000000
0.3704963864575864	0.6295036135424137	0.5000000000000000
0.6295036135424137	0.3704963864575864	0.5000000000000000

Stiffness tensor (GPa):

289.715	92.702	38.980	-0.004	0.023	-0.012
92.702	799.228	164.278	0.011	-0.001	-0.026
38.980	164.278	930.896	0.018	0.004	-0.001
-0.004	0.011	0.018	341.328	0.004	-0.006
0.023	-0.001	0.004	0.004	118.798	0.013
-0.012	-0.026	-0.001	-0.006	0.013	29.942

BN-185

Density (g/cm^3): 2.73 | Space Group: 10

Bulk modulus (GPa): 255 | Shear modulus (GPa): 146

Young's modulus (GPa): 369 | Highest Young's modulus (GPa): 800

Hardness (GPa): 16 | Energy above hull (eV/atom): 0.23

Primitive Cell

1.000000

6.52237292463513	0.00000000000000	0.00000000000000
0.00000000000000	2.54474861947453	0.00000000000000
-0.07993703651899	0.00000000000000	10.92367034859657

B N

12 12

DIRECT

0.7087205895896995	0.0000000000000000	0.9238946459454619
0.2912794104103005	0.0000000000000000	0.0761053540545381
0.1207553444869841	0.0000000000000000	0.8199630250278303
0.8792446555130159	0.0000000000000000	0.1800369749721697
0.2580536136616921	0.0000000000000000	0.4283930936800046
0.7419463863383079	0.0000000000000000	0.5716069063199954
0.2488078807927301	0.5000000000000000	0.6267242183626794
0.7511921192072699	0.5000000000000000	0.3732757816373206
0.2164376423649642	0.5000000000000000	0.2288962545789626
0.7835623576350358	0.5000000000000000	0.7711037454210374
0.3697203384900303	0.5000000000000000	0.8781739494946453
0.6302796615099697	0.5000000000000000	0.1218260505053547
0.2741036468036364	0.0000000000000000	0.9363161397388999
0.7258963531963636	0.0000000000000000	0.0636838602611001
0.2585197682413074	0.0000000000000000	0.5625914000075385
0.7414802317586926	0.0000000000000000	0.4374085999924615
0.1107563814726130	0.0000000000000000	0.1750386316478527
0.8892436185273870	0.0000000000000000	0.8249613683521473
0.2529252881660391	0.5000000000000000	0.3640936574102326
0.7470747118339609	0.5000000000000000	0.6359063425897674
0.6010426228789985	0.5000000000000000	0.8725978960898484
0.3989573771210015	0.5000000000000000	0.1274021039101516
0.2146214335612739	0.5000000000000000	0.7599658384564109
0.7853785664387261	0.5000000000000000	0.2400341615435891

Stiffness tensor (GPa):

367.607	52.916	108.098	0.007	4.317	0.012
52.916	821.688	111.752	0.011	-1.387	0.032
108.098	111.752	705.822	0.020	-13.711	0.029
0.007	0.011	0.020	271.160	-0.004	-5.845
4.317	-1.387	-13.711	-0.004	30.045	-0.007
0.012	0.032	0.029	-5.845	-0.007	147.397

BN-186

Density (g/cm^3): 2.71 | Space Group: 39

Bulk modulus (GPa): 271 | Shear modulus (GPa): 156

Young's modulus (GPa): 393 | Highest Young's modulus (GPa): 856

Hardness (GPa): 17 | Energy above hull (eV/atom): 0.18

Primitive Cell

1.000000

12.13524695166541	0.00000000000000	0.00000000000000
0.00000000000000	3.52220441394785	2.13329125385015
0.00000000000000	-3.52220441394785	2.13329125385015

B N

12 12

DIRECT

0.8554015883085593	0.8838718471307107	0.0925927998906067
0.1445984116914407	0.0925927998906067	0.8838718471307105
0.8554015883085593	0.5925927998906066	0.3838718471307107
0.1445984116914407	0.3838718471307106	0.5925927998906066
0.5528920047142942	0.2558016780155709	0.7558016780155710
0.4471079952857058	0.7558016780155710	0.2558016780155709
0.7673893137052696	0.2367311178756941	0.7367311178756940
0.2326106862947304	0.7367311178756940	0.2367311178756941
0.6536674953825201	0.7588814900447706	0.2588814900447706
0.3463325046174799	0.2588814900447706	0.7588814900447706
0.9387549253512586	0.2370518618004793	0.7370518618004792
0.0612450746487414	0.7370518618004792	0.2370518618004793
0.8548812453006236	0.2619285038610013	0.4486598545994581
0.1451187546993764	0.4486598545994581	0.2619285038610013
0.8548812453006236	0.9486598545994580	0.7619285038610012
0.1451187546993764	0.7619285038610012	0.9486598545994580
0.5512516963725846	0.5913121724462137	0.0913121724462137
0.4487483036274154	0.0913121724462137	0.5913121724462137
0.6559629045222577	0.0908103888638996	0.5908103888638996
0.3440370954777423	0.5908103888638996	0.0908103888638996
0.7620752142901561	0.6035550280375851	0.1035550280375851
0.2379247857098439	0.1035550280375851	0.6035550280375851
0.9455187271884653	0.6058032987499132	0.1058032987499132
0.0544812728115347	0.1058032987499132	0.6058032987499132

Stiffness tensor (GPa):

814.854	49.851	117.102	0.016	-0.004	-0.033
49.851	465.287	34.579	0.026	0.013	0.002
117.102	34.579	874.211	0.016	-0.004	0.107
0.016	0.026	0.016	158.784	-0.002	0.003
-0.004	0.013	-0.004	-0.002	304.145	-0.038
-0.033	0.002	0.107	0.003	-0.038	23.309

BN-187

Density (g/cm^3): 2.56 | Space Group: 84

Bulk modulus (GPa): 232 | Shear modulus (GPa): 144

Young's modulus (GPa): 358 | Highest Young's modulus (GPa): 860

Hardness (GPa): 18 | Energy above hull (eV/atom): 0.18

Primitive Cell

1.000000

8.77041476413872	0.00000000000000	0.00000000000000
0.00000000000000	8.77041476413872	0.00000000000000
0.00000000000000	0.00000000000000	2.51580684947398

B N

12 12

DIRECT

0.8646565382271187	0.3337841560206185	0.0000000000000000
0.1353434617728813	0.6662158439793815	0.0000000000000000
0.6662158439793815	0.8646565382271187	0.5000000000000000
0.3337841560206185	0.1353434617728813	0.5000000000000000
0.4212576595025423	0.8495021052675187	0.0000000000000000
0.5787423404974577	0.1504978947324813	0.0000000000000000
0.1504978947324813	0.4212576595025423	0.5000000000000000
0.8495021052675187	0.5787423404974577	0.5000000000000000
0.0931845797646934	0.1699387173206413	0.0000000000000000
0.9068154202353066	0.8300612826793587	0.0000000000000000
0.8300612826793587	0.0931845797646934	0.5000000000000000
0.1699387173206413	0.9068154202353066	0.5000000000000000
0.8620765160824235	0.6593464277955774	0.0000000000000000
0.1379234839175765	0.3406535722044226	0.0000000000000000
0.3406535722044226	0.8620765160824235	0.5000000000000000
0.6593464277955774	0.1379234839175765	0.5000000000000000
0.0924067209929331	0.8364033975536976	0.0000000000000000
0.9075932790070669	0.1635966024463024	0.0000000000000000
0.1635966024463024	0.0924067209929331	0.5000000000000000
0.8364033975536976	0.9075932790070669	0.5000000000000000
0.4122085361163418	0.1574836609786252	0.0000000000000000
0.5877914638836582	0.8425163390213748	0.0000000000000000
0.8425163390213748	0.4122085361163418	0.5000000000000000
0.1574836609786252	0.5877914638836582	0.5000000000000000

Stiffness tensor (GPa):

460.024	52.420	70.081	0.025	-0.028	-6.965
52.420	459.795	70.071	0.026	0.052	6.834
70.081	70.071	879.228	0.018	0.033	0.032
0.025	0.026	0.018	196.493	0.001	-0.003
-0.028	0.052	0.033	0.001	196.547	0.001
-6.965	6.834	0.032	-0.003	0.001	29.931

BN-188

Density (g/cm^3): 2.50 | Space Group: 105

Bulk modulus (GPa): 255 | Shear modulus (GPa): 148

Young's modulus (GPa): 372 | Highest Young's modulus (GPa): 774

Hardness (GPa): 17 | Energy above hull (eV/atom): 0.25

Primitive Cell

1.000000

4.81959692957341	0.00000000000000	0.00000000000000
0.00000000000000	4.81959692957341	0.00000000000000
0.00000000000000	0.00000000000000	4.25641962033391

B N

6 6

DIRECT

0.0000000000000000	0.2212190015758251	0.6970835386297121
0.0000000000000000	0.7787809984241749	0.6970835386297121
0.7787809984241749	0.0000000000000000	0.1970835386297121
0.2212190015758251	0.0000000000000000	0.1970835386297121
0.0000000000000000	0.5000000000000000	0.1747859852719735
0.5000000000000000	0.0000000000000000	0.6747859852719735
0.0000000000000000	0.2310620245342963	0.3328889974711295
0.0000000000000000	0.7689379754657037	0.3328889974711295
0.7689379754657037	0.0000000000000000	0.8328889974711295
0.2310620245342963	0.0000000000000000	0.8328889974711295
0.0000000000000000	0.5000000000000000	0.8452690422995492
0.5000000000000000	0.0000000000000000	0.3452690422995492

Stiffness tensor (GPa):

586.536	32.360	74.268	0.034	0.024	-0.045
32.360	586.721	74.335	0.032	0.045	0.048
74.268	74.335	791.768	0.022	0.025	0.028
0.034	0.032	0.022	210.016	0.005	-0.009
0.024	0.045	0.025	0.005	210.418	-0.014
-0.045	0.048	0.028	-0.009	-0.014	24.649

BN-189

Density (g/cm^3): 2.40
Space Group: 40
Bulk modulus (GPa): 161
Shear modulus (GPa): 72
Young's modulus (GPa): 189
Highest Young's modulus (GPa): 776
Hardness (GPa): 7
Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

4.98242099412533	0.00000000000000	0.00000000000000
0.00000000000000	1.65356190314321	8.32883466445095
0.00000000000000	-1.65356190314321	8.32883466445095

B N

8 8

DIRECT

0.0000000000000000	0.6085476826832824	0.6085476826832825
0.5000000000000000	0.6085476826832824	0.6085476826832825
0.2500000000000000	0.1025387642500957	0.3411241331666369
0.7500000000000000	0.3411241331666369	0.1025387642500957
0.0000000000000000	0.3475180026418027	0.3475180026418028
0.5000000000000000	0.3475180026418027	0.3475180026418028
0.2500000000000000	0.4811269085728641	0.4746438650222751
0.7500000000000000	0.4746438650222752	0.4811269085728640
0.0000000000000000	0.5218875337935103	0.5218875337935104
0.5000000000000000	0.5218875337935103	0.5218875337935104
0.2500000000000000	0.7715889577867909	0.5285845994005455
0.7500000000000000	0.5285845994005455	0.7715889577867909
0.0000000000000000	0.2607845718340823	0.2607845718340824
0.5000000000000000	0.2607845718340823	0.2607845718340824
0.2500000000000000	0.3759756426038948	0.4069416102680879
0.7500000000000000	0.4069416102680880	0.3759756426038948

Stiffness tensor (GPa):

839.627	22.045	210.813	-0.024	0.041	0.012
22.045	76.964	72.847	-0.039	0.064	0.024
210.813	72.847	703.173	-0.041	0.039	0.029
-0.024	-0.039	-0.041	0.501	0.023	0.006
0.041	0.064	0.039	0.023	246.926	-0.013
0.012	0.024	0.029	0.006	-0.013	25.857

BN-190

Density (g/cm^3): 2.40
Space Group: 1
Bulk modulus (GPa): 150
Shear modulus (GPa): 104
Young's modulus (GPa): 253
Highest Young's modulus (GPa): 874
Hardness (GPa): 17
Energy above hull (eV/atom): 0.01

Primitive Cell

1.000000

2.50789915408464	0.00000000000000	0.00000000000000
-1.25335815505449	2.17246572292442	0.00000000000000
-0.05358397950947	-1.38813231788147	3.15435218272812

B N

1 1

DIRECT

0.0153104701092377	0.2806444841989695	0.8872211333017874
0.3481839409949292	0.9463360539143215	0.8858032458658389

Stiffness tensor (GPa):

918.276	15.389	183.840	61.583	-1.712	4.899
15.389	51.990	65.667	10.168	1.325	1.835
183.840	65.667	781.451	223.327	-1.331	0.116
61.583	10.168	223.327	77.847	0.972	1.404
-1.712	1.325	-1.331	0.972	326.349	99.870
4.899	1.835	0.116	1.404	99.870	40.432

BN-191

Density (g/cm^3): 2.37 | Space Group: 226
Bulk modulus (GPa): 233 | Shear modulus (GPa): 160
Young's modulus (GPa): 390 | Highest Young's modulus (GPa): 413
Hardness (GPa): 22 | Energy above hull (eV/atom): 0.46

Primitive Cell

1.000000

0.00000000000000	5.92946612101994	5.92946612101994
5.92946612101994	0.00000000000000	5.92946612101994
5.92946612101994	5.92946612101994	0.00000000000000

B N

24 24

DIRECT

0.5938213100386871	0.2219938436222526	0.4061786899613130
0.4061786899613130	0.7780061563777473	0.5938213100386871
0.2219938436222526	0.5938213100386870	0.7780061563777474
0.7780061563777474	0.4061786899613129	0.2219938436222526
0.4061786899613129	0.5938213100386871	0.2219938436222526
0.5938213100386871	0.4061786899613130	0.7780061563777474
0.7780061563777474	0.2219938436222526	0.5938213100386871
0.2219938436222526	0.7780061563777474	0.4061786899613129
0.2219938436222526	0.4061786899613130	0.5938213100386871
0.7780061563777474	0.5938213100386871	0.4061786899613129
0.5938213100386871	0.7780061563777474	0.2219938436222526
0.4061786899613129	0.2219938436222526	0.7780061563777474
0.9061786899613129	0.2780061563777474	0.7219938436222526
0.0938213100386870	0.7219938436222526	0.2780061563777474
0.2780061563777474	0.9061786899613129	0.0938213100386871
0.7219938436222526	0.0938213100386871	0.9061786899613129
0.0938213100386871	0.9061786899613129	0.7219938436222525
0.9061786899613129	0.0938213100386871	0.2780061563777474
0.7219938436222526	0.2780061563777474	0.0938213100386870
0.2780061563777474	0.7219938436222526	0.9061786899613129
0.2780061563777475	0.0938213100386870	0.7219938436222526
0.7219938436222526	0.9061786899613129	0.2780061563777474
0.9061786899613129	0.7219938436222526	0.0938213100386872
0.0938213100386871	0.2780061563777474	0.9061786899613129
0.7173649460711622	0.0814376471973182	0.2826350539288380
0.2826350539288380	0.9185623528026817	0.7173649460711620
0.0814376471973183	0.7173649460711620	0.9185623528026818
0.9185623528026818	0.2826350539288379	0.0814376471973183
0.2826350539288380	0.7173649460711621	0.0814376471973182
0.7173649460711621	0.2826350539288380	0.9185623528026818
0.9185623528026818	0.0814376471973183	0.7173649460711621
0.0814376471973183	0.9185623528026818	0.2826350539288379
0.0814376471973182	0.2826350539288380	0.7173649460711621

0.9185623528026817	0.7173649460711622	0.2826350539288380
0.7173649460711620	0.9185623528026817	0.0814376471973184
0.2826350539288380	0.0814376471973183	0.9185623528026818
0.7826350539288380	0.4185623528026818	0.5814376471973184
0.2173649460711621	0.5814376471973184	0.4185623528026818
0.4185623528026817	0.7826350539288379	0.2173649460711621
0.5814376471973182	0.2173649460711621	0.7826350539288380
0.2173649460711620	0.7826350539288380	0.5814376471973183
0.7826350539288379	0.2173649460711621	0.4185623528026817
0.5814376471973184	0.4185623528026818	0.2173649460711620
0.4185623528026817	0.5814376471973184	0.7826350539288380
0.4185623528026818	0.2173649460711620	0.5814376471973184
0.5814376471973184	0.7826350539288379	0.4185623528026818
0.7826350539288380	0.5814376471973182	0.2173649460711620
0.2173649460711620	0.4185623528026817	0.7826350539288379

Stiffness tensor (GPa):

424.640	137.053	137.056	-0.012	-0.000	0.008
137.053	424.628	137.063	-0.003	0.001	0.002
137.056	137.063	424.633	-0.006	-0.002	-0.000
-0.012	-0.003	-0.006	171.294	0.002	0.016
-0.000	0.001	-0.002	0.002	171.274	-0.028
0.008	0.002	-0.000	0.016	-0.028	171.319

BN-192

Density (g/cm^3): 2.30 | Space Group: 8
Bulk modulus (GPa): 205 | Shear modulus (GPa): 122
Young's modulus (GPa): 306 | Highest Young's modulus (GPa): 819
Hardness (GPa): 15 | Energy above hull (eV/atom): 0.13

Primitive Cell

1.000000

6.53521040884693	-1.25480781531531	0.00000000000000
6.53521040884693	1.25480781531531	0.00000000000000
-0.09912435499554	0.00000000000000	4.37537262906726

B N

4 4

DIRECT

0.0000300166094667	0.0000300166094666	0.9987383734118285
0.2000695210272543	0.2000695210272542	0.4292537827161762
0.8655874769449849	0.8655874769449849	0.3779529417004767
0.5316413141718224	0.5316413141718221	0.4991984380805085
0.9806208202785535	0.9806208202785534	0.3423838152203322
0.5063540834531799	0.5063540834531799	0.8432614146066761
0.6470361963164277	0.6470361963164277	0.4470945625851119
0.3121605754029486	0.3121605754029484	0.3907166314436061

Stiffness tensor (GPa):

547.245	100.680	56.511	0.090	-44.768	0.021
100.680	843.695	53.379	0.051	-13.928	0.046
56.511	53.379	330.975	-0.014	-22.254	0.139
0.090	0.051	-0.014	132.310	0.012	-16.470
-44.768	-13.928	-22.254	0.012	24.397	-0.003
0.021	0.046	0.139	-16.470	-0.003	214.944

BN-193

Density (g/cm^3): 2.10 | Space Group: 228

Bulk modulus (GPa): 217 | Shear modulus (GPa): 95

Young's modulus (GPa): 248 | Highest Young's modulus (GPa): 314

Hardness (GPa): 8 | Energy above hull (eV/atom): 0.16

Primitive Cell

1.000000

0.00000000000000	6.17501074345986	6.17501074345986
6.17501074345986	0.00000000000000	6.17501074345986
6.17501074345986	6.17501074345986	0.00000000000000

N B

24 24

DIRECT

0.1250000000000000	0.7897839222460825	0.4602160777539175
0.7897839222460825	0.1250000000000000	0.6250000000000000
0.4602160777539175	0.6250000000000000	0.1250000000000000
0.6250000000000000	0.4602160777539175	0.7897839222460825
0.4602160777539175	0.1250000000000000	0.7897839222460825
0.6250000000000000	0.7897839222460825	0.1250000000000000
0.1250000000000000	0.4602160777539175	0.6250000000000000
0.7897839222460825	0.6250000000000000	0.4602160777539175
0.7897839222460825	0.4602160777539175	0.1250000000000000
0.1250000000000000	0.6250000000000000	0.7897839222460825
0.6250000000000000	0.1250000000000000	0.4602160777539175
0.4602160777539175	0.7897839222460825	0.6250000000000000
0.6250000000000000	0.9602160777539175	0.2897839222460825
0.9602160777539175	0.6250000000000000	0.1250000000000000
0.2897839222460825	0.1250000000000000	0.6250000000000000
0.1250000000000000	0.2897839222460825	0.9602160777539175
0.2897839222460825	0.6250000000000000	0.9602160777539175
0.1250000000000000	0.9602160777539175	0.6250000000000000
0.6250000000000000	0.2897839222460825	0.1250000000000000
0.9602160777539175	0.1250000000000000	0.2897839222460825
0.9602160777539175	0.2897839222460825	0.6250000000000000
0.6250000000000000	0.1250000000000000	0.9602160777539175
0.1250000000000000	0.6250000000000000	0.2897839222460825
0.2897839222460825	0.9602160777539175	0.1250000000000000
0.1250000000000000	0.4601611120358626	0.7898388879641374
0.4601611120358626	0.1250000000000000	0.6250000000000000
0.7898388879641374	0.6250000000000000	0.1250000000000000
0.6250000000000000	0.7898388879641374	0.4601611120358626
0.7898388879641374	0.1250000000000000	0.4601611120358626
0.6250000000000000	0.4601611120358626	0.1250000000000000
0.1250000000000000	0.7898388879641374	0.6250000000000000
0.4601611120358626	0.6250000000000000	0.7898388879641374
0.4601611120358626	0.7898388879641374	0.1250000000000000

0.1250000000000000	0.6250000000000000	0.4601611120358626
0.6250000000000000	0.1250000000000000	0.7898388879641374
0.7898388879641374	0.4601611120358626	0.6250000000000000
0.6250000000000000	0.2898388879641374	0.9601611120358626
0.2898388879641374	0.6250000000000000	0.1250000000000000
0.9601611120358626	0.1250000000000000	0.6250000000000000
0.1250000000000000	0.9601611120358626	0.2898388879641374
0.9601611120358626	0.6250000000000000	0.2898388879641374
0.1250000000000000	0.2898388879641374	0.6250000000000000
0.6250000000000000	0.9601611120358626	0.1250000000000000
0.2898388879641374	0.1250000000000000	0.9601611120358626
0.2898388879641374	0.9601611120358626	0.6250000000000000
0.6250000000000000	0.1250000000000000	0.2898388879641374
0.1250000000000000	0.6250000000000000	0.9601611120358626
0.9601611120358626	0.2898388879641374	0.1250000000000000

Stiffness tensor (GPa):

300.529	175.182	175.190	0.043	0.004	0.021
175.182	300.477	175.174	-0.010	0.055	0.009
175.190	175.174	300.512	0.014	0.004	0.054
0.043	-0.010	0.014	124.923	0.006	-0.006
0.004	0.055	0.004	0.006	124.923	-0.009
0.021	0.009	0.054	-0.006	-0.009	124.919

BN-194

Density (g/cm^3): 1.86 | Space Group: 187

Bulk modulus (GPa): 186 | Shear modulus (GPa): 55

Young's modulus (GPa): 149 | Highest Young's modulus (GPa): 494

Hardness (GPa): 2 | Energy above hull (eV/atom): 0.45

Primitive Cell

1.000000

6.39016150160460	0.00000000000000	0.00000000000000
-3.19508075080230	5.53404219467490	0.00000000000000
0.00000000000000	0.00000000000000	2.50592950169361

B N

4 4

DIRECT

0.5335143039179979	0.4664856960820022	0.0000000000000000
0.5335143039179979	0.0670286078359956	0.0000000000000000
0.9329713921640044	0.4664856960820022	0.0000000000000000
0.3333333333333333	0.6666666666666666	0.5000000000000000
0.4681608000070391	0.5318391999929608	0.5000000000000000
0.4681608000070391	0.9363216000140784	0.5000000000000000
0.0636783999859216	0.5318391999929608	0.5000000000000000
0.6666666666666667	0.3333333333333333	0.0000000000000000

Stiffness tensor (GPa):

239.895	181.242	86.551	0.138	0.115	-0.038
181.242	240.327	82.867	0.060	0.127	-0.008
86.551	82.867	527.752	0.271	0.538	0.530
0.138	0.060	0.271	43.810	0.001	-0.009
0.115	0.127	0.538	0.001	43.564	-0.037
-0.038	-0.008	0.530	-0.009	-0.037	29.644

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