Thermodynamic stability of hexagonal and rhombohedral boron nitride under chemical vapor deposition conditions from van der Waals corrected first principles calculations

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Thermodynamic stability of hexagonal and rhombohedral BN at CVD conditions from van der Waals corrected first principles calculations

Running title: Stability of h-BN and r-BN at CVD conditions

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Thin films of boron nitride (BN), particularly the sp^2 -hybridized polytypes hexagonal BN (h-BN) and rhombohedral BN (r-BN) are interesting for several electronic applications given band gaps in the UV. They are typically deposited close to thermal equilibrium by chemical vapor deposition (CVD) at temperatures and pressures in the regions 1400-1800 K and 1000-10000 Pa, respectively. In this letter, we use van der Waals corrected density functional theory and thermodynamic stability calculations to determine the stability of r-BN and compare it to that of h-BN as well as to cubic BN and wurtzitic BN. We find that r-BN is the stable sp^2 -hybridized phase at CVD conditions, while h-BN is metastable. Thus, our calculations suggest that thin films of h-BN must be deposited far from thermal equilibrium.

I. INTRODUCTION

Cubic BN (c-BN) with sp^3 -hybridization and diamond structure is the most well-known among BN phases. In 1957, Wentorf synthesized c-BN from a mixture of boron and nitrogen at high temperature and pressures.¹ The discovery of “Borazon” catalyzed work on the other polytypes of BN, foremost sp^2 -hybridized hexagonal BN (h-BN) “white graphite” and to some extent the less studied wurtzite form (w-BN) that is similar to “hexagonal diamond”. In addition to h-BN a rhombohedral sp^2 -hybridized BN phase (r-BN) was reported 1958 by Hérol.² The two sp^2 -hybridized BN polytypes differ in their stacking sequence of the basal planes along the c-axis; h-BN exhibits an ABAB... stacking while r-BN has an ABCABC... stacking sequence.³ Furthermore, the basal planes in h-BN are rotated 180° , with respect to the previous basal plane, around the c-axis ([0001]), while in r-BN, each next basal plane is instead shifted along the $[1\bar{1}00]$ direction by $1.45 \text{ \AA}$. The very close structural similarity between h-BN and r-BN is demonstrated in identical in-plane lattice parameters, $2.504 \text{ \AA}$, and spacing between the basal planes, $3.333 \text{ \AA}$.⁴

As a thin film, BN is a promising material for many electronic applications,⁵⁻⁸ where the polytype, h-BN or r-BN, are likely to affect the electronic properties: h-BN is reported to have a slightly larger band gap than r-BN; 5.955^9 and 5.7^{10} eV , respectively. Typically, sp^2 -BN films have been deposited by thermally activated Chemical Vapor Deposition (CVD), i.e. close to thermal equilibrium conditions. Epitaxial growth of sp^2 -BN thin films by CVD is typically carried out from triethylboron, $B(C_2H_5)_3$ (TEB), and ammonia, NH_3 at low pressures of $1000 - 10000 \text{ Pa}$ and temperatures in the range of $1100-1500 \text{ }^\circ\text{C}$ ($1400-1800 \text{ K}$).¹¹ The high temperatures needed limit the number of available substrate materials, thus, growth of epitaxial films has been restricted to α - Al_2O_3 (0001) and 4H/6H-SiC (0001) substrates, yielding films oriented around the c-axis.¹²⁻¹⁵ sp^2 -BN as a two-dimensional material will consist of a single basal plane with hexagonal symmetry and it is therefore, correctly, refer to as h-BN. However, the authors have previously pointed out the difficulty in structural determination of sp^2 -BN films grown along the c-axis, i.e. the [0001] direction, of thicknesses exceeding a few

nanometers, and advised to use a more extensive characterization approach to fully understand if a film of sp^2 -BN is h-BN or r-BN.³

In this letter, the authors use van der Waals corrected density functional theory and thermodynamic stability calculations to study the stability of the sp^2 -BN polytypes at temperatures and pressures relevant to CVD. From the results it is found that at typical CVD temperatures and pressures, r-BN is the phase predicted to be most stable by thermodynamics.

II. COMPUTATIONAL DETAILS

A. *First-principles calculations*

The first principles total energies E_0 at $T = 0$ K as a function of volume V of the four BN polytypes are derived from the density functional theory (DFT),^{16, 17} in which the project augmented wave (PAW) method¹⁸, as implemented in the Vienna ab initio simulation package (VASP),^{19, 20} is used and the generalized gradient approximation (GGA), as proposed by Perdew, Burke, and Ernzerhof²¹, is employed for modeling the exchange-correlation interactions. For the four BN polytypes, the energy cutoff for plane waves, included in the expansion of wave functions, is set to 600 eV, and the Monkhorst-Pack k-point mesh²² of $15 \times 15 \times 15$ is chosen for the Brillouin zone integration. Since the standard DFT calculations cannot accurately describe the van der Waals interactions, the DFT-D3 correction method with Becke-Jonson damping^{23, 24} is used to account for the interactions. For each BN polytype, the optimal equilibrium volume V_0 at $T = 0$ K, minimizing E_0 , is determined by the minimum point of the total energy curve $E_0(V)$, calculated for a set of different fixed V . During the calculations of E_0 at each fixed V , the unit-cell shape and all internal atomic coordinates within the cell are fully relaxed so that the total force, acting on each atom, is less than 10^{-6} eV/Å. Note that, for this particular case, the calculated $E_0(V)$ are all assured to be converged within an accuracy of 1 meV/atom with respect to both the energy cutoff and the number of k-points.

B. *Thermodynamic stability calculations*

The relative thermodynamic stability of the four BN polytypes at different fixed pressures p and temperature T is evaluated by minimization of the Gibbs free energy $G(T, p)$:

$$G(T, p) = E_0(V) + F_{vib}(T, V) + pV, \quad (1)$$

where $E_0(V)$ is the total energy at $T = 0$ directly obtained from the DFT calculations, as described in section II A. $F_{vib}(T, V)$ is the Helmholtz free energy contributed by the lattice vibrations (phonons), given by;

$$F_{vib}(T, V) = \frac{1}{2} \sum_{\mathbf{q}, \nu} \hbar \omega(\mathbf{q}, \nu, V) + k_B T \sum_{\mathbf{q}, \nu} \ln(1 - e^{-\hbar \omega(\mathbf{q}, \nu, V)/k_B T}). \quad (2)$$

$\omega(\mathbf{q}, \nu, V)$ is the phonon frequency at the wave vector $\mathbf{q}$ and the band index ν . $\hbar$ and k_B are the reduced Planck constant and the Boltzmann constant, respectively. It is worth noting that, in addition to $\mathbf{q}$ and ν , the phonon frequencies ω in Eq. 2 are volume dependent, as the phonon calculations are performed at the quasi-harmonic level using the PHONOPY package for phonon calculations^{25, 26}, in which the Parlinski-Li-Kawazoe method²⁷ with a finite displacement of 0.01 Å is used to calculate the force constants within sufficiently large supercells, i.e., $4 \times 4 \times 1$ primitive hexagonal unit cells for h-BN (64 atoms), $4 \times 4 \times 1$ conventional hexagonal unit cells for r-BN (96 atoms), $2 \times 2 \times 2$ conventional cubic unit cells for c-BN (64 atoms), and $3 \times 3 \times 3$ primitive hexagonal unit cells for w-BN (108 atoms). The supercells are then sampled with the $21 \times 21 \times 21$ Monkhorst-Pack $\mathbf{q}$ -point grids in order to secure the convergence of the phonon frequencies and thus $F_{vib}(T, V)$. To determine the term pV and include it in $G(T, p)$ at fixed temperatures, the sums of the first two terms on the right-hand side of Eq. 1 at different fixed volumes are fitted to the third-order Birch-Murnaghan equation of state (EOS)^{28, 29}. The pressure p is thus calculated by;

$$p = - \left[\frac{\partial [E_0(V) + F_{vib}(T, V)]}{\partial V} \right]_T. (3)$$

III. RESULTS

From minimization of the calculated Gibbs free energy $G(T, p)$ and the methodology described in section II, p - T phase diagrams were constructed to determine the relative thermodynamic stability of the BN polytypes, h-BN, r-BN, c-BN and w-BN. Fig. 1(a) shows the relative thermodynamic stability between h-BN and r-BN, excluding formation of c-BN and w-BN. As can be seen r-BN is stable at p - T conditions typical for CVD, i.e. below atmospheric pressure 0.1 GPa (1013 hPa) and temperatures below 1900 K. h-BN is stable at much higher pressures starting at about 12 GPa and where the h-BN to r-BN transition temperature decreases as the pressure increases.

Fig. 1 Calculated p - T phase diagrams at a composition of BN, illustrating (a) the relative thermodynamic stability between r-BN and h-BN and (b) the thermodynamic stability of boron nitride, including the four polytypes, r-BN, h-BN, c-BN, and w-BN. The insert in Fig 1 b highlights for clarity the stabilities of r-BN and c-BN in the low-temperature and low-pressure region. For completeness are error bars, indicating the consequence of an inherent ± 1 meV/atom uncertainty of the numerical parameters in the method, included.

Fig. 1(b) illustrates the relative thermodynamic stability between the polytypes, r-BN, h-BN, c-BN, and w-BN at p ranging from 0 to 6 GPa. At $T = 0$ K and p 0.1 GPa (atmospheric pressure), r-BN is suggested to undergo the structural phase transformation to c-BN. At $T > 300$ K, the r-BN-to-c-BN transition pressure increases almost linearly with increasing temperature seen from $T = 300$ K where the transformation from r-BN to c-BN takes place at $p = 0.4$ GPa, while the transition pressure increases to 5.7 GPa at $T = 2400$ K. From these calculations, it is evident that although considered, neither h-BN nor w-BN was found to be thermodynamically favored at the investigated temperatures and pressures.

From the phonon density of states (PDOS) of r-BN, h-BN, c-BN and w-BN in (Fig. 2), it is seen that their phonon frequencies are all positive, thus confirming the dynamical stabilities of all polytypes. It is also worth mentioning that our derived PDOS is found to well match those previously reported by Yu et al.³⁰ and Kern et al.³¹ in terms of both phonon frequencies and features of corresponding density of states. This strengthens the reliability of our theoretical prediction.

Fig. 2 Phonon density of states (PDOS) of (a) r-BN, (b) h-BN, (c) c-BN, and (d) w-BN.

The optimized lattice parameters of r-BN, h-BN and c-BN as a function of temperature were derived from the quasiharmonic approximation (Fig. 3). At $T = 300$ K, the lattice parameters a and c of r-BN are 2.509 Å and 10.089 Å, respectively, and the lattice parameter a of c-BN is 3.623 Å. As can be seen from Table 1, our theoretical values derived in the present work are found to differ from the experimental ones, measured at room temperature, by less than 1 %³²⁻³⁴. Thus, our theoretical calculations are in good agreement with the experimental data. It is worth noting that as the temperature increases from 300 K to 2400 K the isotropic c-BN lattice expands 0.05 Å, (1.3 %) while the anisotropic r-BN and h-BN lattices expands 0.4 Å (4 %) and 0.03 Å (0.4 %), respectively in the c -direction, but only 0.004 Å (0.16 %) and 0.001 Å (0.04 %), respectively, in the a -direction. This is a signature of strong B-N bonds within the sp^2 -hybridized basal planes.

Fig. 3 Optimized lattice parameters of r-BN, h-BN and c-BN as a function of temperature.

From Fig. 3 an anomalous feature in the lattice parameters of h-BN can be noted at about 600 K, where the lattice parameter a contracts and then barely expands at higher temperature. The contraction may be interpreted as the negative thermal expansion coefficient in the a -axis, previously reported for h-BN.³⁵

Table 1 Lattice parameters of r-BN and c-BN at $T = 300$ K, calculated in the present work. Comparison is made with the existing experimental data, reported in the literature.³²⁻³⁴

	a (Å)	c (Å)	Reference
r-BN	2.509	10.089	This work
	2.506	10.03	(32)
	2.504	9.99	(34)
h-BN	2.506	6.617	This work
	2.504	6.656	(34)
c-BN	3.623	-	This work
	3.616	-	(33)
	3.615	-	(34)

IV. DISCUSSION

Our calculations show that of the four BN polytypes, r-BN is the most thermodynamically stable at typical CVD conditions; $T = 1400$ - 1800 K and $p = 1000$ - $10\,000$ Pa, see Fig. 1(b). This is supported by experimental studies by Solozhenko et al.³⁶ The relative thermodynamic stability of the four BN polytypes previously derived from first-principles approach by Yu et al.³⁰ and Solozhenko et al.³⁷ suggested c-BN to be the most thermodynamically stable phase at ambient conditions. We attribute this discrepancy to our results to be a consequence of the inclusion of correction factors for long-range van der Waals interactions between the BN sheets in the sp^2 -hybridized

polytypes h-BN and r-BN. These corrections were not included in Ref. (30). Furthermore, it has been demonstrated that standard DFT calculations fail to provide an appropriate description of the van der Waals interactions, which is important for explaining the properties, e.g., interlayer distance and binding energy, of layered materials like graphite³⁸ and h-BN^{39, 40}.

In order to support that the thermodynamic stability of r-BN, predicted in the presented work, does not arise from the use of particular van der Waals correction methods, we evaluate the relative stability between r-BN and h-BN at $T = 0$ K without the inclusion of the phonon zero-point motion by using different correction methods, i.e., DFT-D2⁴¹ and DFT-TS^{42, 43} methods. We find that in all cases r-BN is predicted to be thermodynamically favored over h-BN, indicating that our results are qualitatively robust regardless of which van der Waals correction method is used. Yu et al.³⁰ investigated, apart from the relative stability, different possible transformation paths among the four polytypes of boron nitride. They demonstrated that the direct martensitic transformation between r-BN and c-BN exhibits the smallest energy barrier. As compared to that of r-BN, the direct martensitic transformation between h-BN and c-BN is far less favorable, and an intermediate phase, i.e., r-BN or w-BN, is essentially needed to facilitate such a transformation to c-BN. Even though nucleation and growth-type processes should be considered in the transformation studies, nevertheless, their results support the results presented here that r-BN and c-BN are the only thermodynamically stable phases of boron nitride, thus appearing on the phase diagram depicted in Fig. 1(b), while h-BN and w-BN may merely be metastable polytypes of BN.

The results in this study suggest r-BN to be the most favorable BN polytype at typical conditions for CVD of sp^2 -BN films, 1000 – 10000 Pa and 1100-1500 °C (1400-1800 K). As thermally activated CVD is at thermal equilibrium, the results presented here yield questions for the conditions at which h-BN can be deposited. The authors have shown that phase determination of 0001 oriented sp^2 -BN films require advanced thin film X-ray diffraction techniques; glancing incidence diffraction of asymmetric peaks with 2θ angles unique for each structure and pole figure measurements.³ The authors have reported CVD of h-BN using α -Al₂O₃ (0001) with a strained AlN buffer layer as substrate at 1500 °C and 7000 Pa.⁴⁴ These conditions yielded a polytype pure h-BN film

of 4 nm before the h-BN stacking altered to that in r-BN and where r-BN grew to a total film thickness of 200 nm. The change in polytype was suggested to depend on lattice-mismatch-induced stress relaxation. As comparison, growth on 6H-SiC (0001) substrates resulted in a 200 nm as phase pure r-BN film, using the same CVD process conditions as on α -Al₂O₃ (0001).

From our calculations, it seems that the growth of h-BN as a thin film material must be conducted far from thermal equilibrium, highlighting deposition techniques such as sputtering or possibly plasma CVD. From our previously reported growth results, the choice of substrate for h-BN seems critical and the available thickness achievable seems limited. Our calculations indicate that the h-BN lattice seems to be less liable to expansion than the r-BN lattice from our results on thermal expansion of the lattices, indicating that r-BN is less sensitive to lattice mismatch to the substrate. All these conditions are met in the study by Sutter et al.⁴⁵, presenting epitaxial growth of h-BN on Al₂O₃(0001) substrates with an in-situ epitaxially grown 100 nm Ru(0001) seed layer, using reactive radio frequency magnetron sputtering of a boron target in a nitrogen containing plasma at a temperature of 850 °C. The h-BN films could be deposited to a thickness of approximately 10 BN layers. This corresponds to five unit cells in the c-direction and 3.3 nm, which is close to the 4 nm reported from growth by CVD by the authors⁴⁴.

V. SUMMARY

From van der Waals corrected density functional theory and thermodynamic stability calculations it is found that r-BN is the most stable BN polytype at conditions typically employed for CVD of sp²-BN thin films, 1100-1500 °C and 1000-10 000 Pa, suggesting that deposition of h-BN films must be done far from thermal equilibrium. It is also found that the h-BN lattice less liable to expansion than the r-BN lattice and therefore likely to be more sensitive to lattice mismatch to the substrate.

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Supplementary Information

Thermodynamic stability of hexagonal and rhombohedral BN at CVD conditions from van der Waals corrected first principles calculations

Running title: Stability of h-BN and r-BN at CVD conditions

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Supplementary Figure S1

Figure S1: Vibrational free energies (F_{vib}) of c-BN, derived from $2 \times 2 \times 2$ (red line) and $3 \times 3 \times 3$ (blue dashed line) conventional cubic unit cells. The inset represents the free energy difference between the two model sizes.

Supplementary Information: Gibbs free energy difference

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference **at a given temperature of 0 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.005286002	0.00046129	0.017516986
0.1	0	0.005213269	-0.001502839	0.015562396
0.2	0	0.005142388	-0.003447442	0.013627333
0.3	0	0.005073255	-0.005373243	0.011711072
0.4	0	0.005005775	-0.00728091	0.009812944
0.5	0	0.004939863	-0.009171063	0.007932329
0.6	0	0.004875443	-0.01104428	0.00606865
0.7	0	0.004812444	-0.0129011	0.004221368
0.8	0	0.0047508	-0.014742025	0.00238998
0.9	0	0.004690454	-0.016567528	0.000574014
1	0	0.00463135	-0.018378053	-0.001226975
1.1	0	0.004573437	-0.020174018	-0.003013404
1.2	0	0.004516668	-0.021955818	-0.004785669
1.3	0	0.004461	-0.023723827	-0.006544142
1.4	0	0.004406392	-0.025478398	-0.008289178
1.5	0	0.004352806	-0.027219866	-0.010021112
1.6	0	0.004300207	-0.028948551	-0.011740263
1.7	0	0.00424856	-0.030664755	-0.013446935
1.8	0	0.004197835	-0.032368769	-0.015141416
1.9	0	0.004148001	-0.034060868	-0.016823982
2	0	0.004099032	-0.035741315	-0.018494898
2.1	0	0.004050901	-0.037410363	-0.020154415
2.2	0	0.004003582	-0.039068254	-0.021802775
2.3	0	0.003957052	-0.040715218	-0.023440209
2.4	0	0.003911289	-0.042351477	-0.025066939

2.5	0	0.003866271	-0.043977246	-0.026683178
2.6	0	0.003821979	-0.045592728	-0.028289131
2.7	0	0.003778393	-0.047198121	-0.029884996
2.8	0	0.003735494	-0.048793615	-0.031470963
2.9	0	0.003693265	-0.050379392	-0.033047213
3	0	0.00365169	-0.051955629	-0.034613924
3.1	0	0.003610753	-0.053522497	-0.036171265
3.2	0	0.003570437	-0.055080158	-0.037719402
3.3	0	0.003530729	-0.056628774	-0.039258492
3.4	0	0.003491614	-0.058168495	-0.04078869
3.5	0	0.00345308	-0.059699472	-0.042310144
3.6	0	0.003415112	-0.061221848	-0.043822997
3.7	0	0.003377699	-0.062735763	-0.045327389
3.8	0	0.003340829	-0.064241351	-0.046823456
3.9	0	0.00330449	-0.065738743	-0.048311327
4	0	0.003268671	-0.067228067	-0.04979113
4.1	0	0.003233362	-0.068709445	-0.051262988
4.2	0	0.003198552	-0.070182997	-0.052727021
4.3	0	0.003164231	-0.071648839	-0.054183346
4.4	0	0.003130389	-0.073107086	-0.055632074
4.5	0	0.003097019	-0.074557846	-0.057073317
4.6	0	0.003064109	-0.076001226	-0.05850718
4.7	0	0.003031653	-0.07743733	-0.059933769
4.8	0	0.002999641	-0.07886626	-0.061353184
4.9	0	0.002968066	-0.080288115	-0.062765524
5	0	0.002936919	-0.08170299	-0.064170885
5.1	0	0.002906194	-0.08311098	-0.065569362
5.2	0	0.002875882	-0.084512174	-0.066961044
5.3	0	0.002845977	-0.085906664	-0.068346022
5.4	0	0.002816471	-0.087294535	-0.069724382
5.5	0	0.002787359	-0.088675873	-0.071096209
5.6	0	0.002758633	-0.09005076	-0.072461587

5.7	0	0.002730287	-0.091419276	-0.073820595
5.8	0	0.002702315	-0.092781502	-0.075173313
5.9	0	0.002674711	-0.094137515	-0.076519818
6	0	0.00264747	-0.095487389	-0.077860185
6.1	0	0.002620585	-0.096831199	-0.079194489
6.2	0	0.002594051	-0.098169017	-0.080522802
6.3	0	0.002567863	-0.099500912	-0.081845193
6.4	0	0.002542015	-0.100826956	-0.083161733
6.5	0	0.002516503	-0.102147214	-0.084472488
6.6	0	0.002491322	-0.103461753	-0.085777525
6.7	0	0.002466466	-0.104770638	-0.087076909
6.8	0	0.002441931	-0.106073933	-0.088370703
6.9	0	0.002417713	-0.107371698	-0.089658969
7	0	0.002393807	-0.108663997	-0.090941768
7.1	0	0.002370209	-0.109950887	-0.09221916
7.2	0	0.002346914	-0.111232428	-0.093491204
7.3	0	0.002323918	-0.112508676	-0.094757956
7.4	0	0.002301217	-0.113779689	-0.096019473
7.5	0	0.002278808	-0.115045521	-0.09727581
7.6	0	0.002256686	-0.116306226	-0.098527021
7.7	0	0.002234848	-0.117561858	-0.09977316
7.8	0	0.00221329	-0.118812469	-0.101014278
7.9	0	0.002192008	-0.120058109	-0.102250426
8	0	0.002170999	-0.121298829	-0.103481656
8.1	0	0.002150259	-0.122534678	-0.104708015
8.2	0	0.002129785	-0.123765705	-0.105929553
8.3	0	0.002109574	-0.124991957	-0.107146317
8.4	0	0.002089622	-0.126213481	-0.108358354
8.5	0	0.002069927	-0.127430323	-0.109565709
8.6	0	0.002050485	-0.128642528	-0.110768429
8.7	0	0.002031293	-0.12985014	-0.111966556
8.8	0	0.002012348	-0.131053203	-0.113160135

8.9	0	0.001993648	-0.13225176	-0.114349209
9	0	0.001975189	-0.133445853	-0.11553382
9.1	0	0.001956968	-0.134635523	-0.116714008
9.2	0	0.001938984	-0.13582081	-0.117889816
9.3	0	0.001921233	-0.137001757	-0.119061283
9.4	0	0.001903712	-0.1381784	-0.120228448
9.5	0	0.001886419	-0.13935078	-0.12139135
9.6	0	0.001869352	-0.140518935	-0.122550028
9.7	0	0.001852508	-0.141682901	-0.123704519
9.8	0	0.001835884	-0.142842717	-0.124854861
9.9	0	0.001819478	-0.143998419	-0.126001088
10	0	0.001803289	-0.145150042	-0.127143238
10.1	0	0.001787312	-0.146297622	-0.128281346
10.2	0	0.001771548	-0.147441193	-0.129415447
10.3	0	0.001755991	-0.14858079	-0.130545574
10.4	0	0.001740642	-0.149716447	-0.131671762
10.5	0	0.001725498	-0.150848197	-0.132794043
10.6	0	0.001710556	-0.151976072	-0.133912452
10.7	0	0.001695814	-0.153100106	-0.135027019
10.8	0	0.001681272	-0.154220328	-0.136137776
10.9	0	0.001666925	-0.155336772	-0.137244756
11	0	0.001652773	-0.156449468	-0.138347989
11.1	0	0.001638814	-0.157558447	-0.139447505
11.2	0	0.001625045	-0.158663738	-0.140543335
11.3	0	0.001611465	-0.159765371	-0.141635507
11.4	0	0.001598073	-0.160863375	-0.142724052
11.5	0	0.001584865	-0.16195778	-0.143808998
11.6	0	0.001571841	-0.163048612	-0.144890374
11.7	0	0.001558998	-0.164135902	-0.145968207
11.8	0	0.001546336	-0.165219676	-0.147042526
11.9	0	0.001533851	-0.166299961	-0.148113357
12	0	0.001521544	-0.167376784	-0.149180727

12.1	0	0.001509411	-0.168450173	-0.150244663
12.2	0	0.001497451	-0.169520153	-0.151305192
12.3	0	0.001485663	-0.170586749	-0.152362338
12.4	0	0.001474046	-0.171649988	-0.153416128
12.5	0	0.001462597	-0.172709895	-0.154466587
12.6	0	0.001451315	-0.173766494	-0.15551374
12.7	0	0.001440199	-0.174819811	-0.15655761
12.8	0	0.001429247	-0.175869869	-0.157598223
12.9	0	0.001418458	-0.176916692	-0.158635603
13	0	0.00140783	-0.177960304	-0.159669772
13.1	0	0.001397362	-0.179000729	-0.160700755
13.2	0	0.001387052	-0.180037988	-0.161728574
13.3	0	0.0013769	-0.181072106	-0.162753252
13.4	0	0.001366903	-0.182103105	-0.163774812
13.5	0	0.001357061	-0.183131006	-0.164793276
13.6	0	0.001347372	-0.184155832	-0.165808666
13.7	0	0.001337835	-0.185177605	-0.166821003
13.8	0	0.001328448	-0.186196345	-0.167830309
13.9	0	0.001319211	-0.187212074	-0.168836606
14	0	0.001310122	-0.188224814	-0.169839913
14.1	0	0.00130118	-0.189234584	-0.170840252
14.2	0	0.001292384	-0.190241405	-0.171837644
14.3	0	0.001283732	-0.191245297	-0.172832107
14.4	0	0.001275223	-0.192246281	-0.173823664
14.5	0	0.001266857	-0.193244375	-0.174812332
14.6	0	0.001258632	-0.1942396	-0.175798131
14.7	0	0.001250546	-0.195231975	-0.176781082
14.8	0	0.0012426	-0.196221519	-0.177761203
14.9	0	0.001234791	-0.19720825	-0.178738512
15	0	0.001227119	-0.198192188	-0.179713029
15.1	0	0.001219583	-0.19917335	-0.180684772
15.2	0	0.001212181	-0.200151756	-0.181653759

15.3	0	0.001204913	-0.201127422	-0.182620008
15.4	0	0.001197777	-0.202100368	-0.183583538
15.5	0	0.001190773	-0.203070609	-0.184544365
15.6	0	0.001183899	-0.204038165	-0.185502507
15.7	0	0.001177154	-0.205003053	-0.186457981
15.8	0	0.001170539	-0.205965288	-0.187410805
15.9	0	0.00116405	-0.206924889	-0.188360995
16	0	0.001157689	-0.207881871	-0.189308569
16.1	0	0.001151453	-0.208836252	-0.190253542
16.2	0	0.001145342	-0.209788048	-0.191195931
16.3	0	0.001139355	-0.210737275	-0.192135752
16.4	0	0.001133491	-0.211683949	-0.193073022
16.5	0	0.001127749	-0.212628086	-0.194007756
16.6	0	0.001122128	-0.213569702	-0.194939969
16.7	0	0.001116627	-0.214508811	-0.195869678
16.8	0	0.001111246	-0.215445431	-0.196796898
16.9	0	0.001105983	-0.216379575	-0.197721643
17	0	0.001100839	-0.217311259	-0.19864393
17.1	0	0.001095811	-0.218240497	-0.199563772
17.2	0	0.001090899	-0.219167305	-0.200481185
17.3	0	0.001086103	-0.220091698	-0.201396184
17.4	0	0.001081421	-0.221013689	-0.202308782
17.5	0	0.001076853	-0.221933292	-0.203218995
17.6	0	0.001072398	-0.222850523	-0.204126836
17.7	0	0.001068055	-0.223765395	-0.205032319
17.8	0	0.001063823	-0.224677923	-0.205935459
17.9	0	0.001059703	-0.225588119	-0.206836269
18	0	0.001055692	-0.226495998	-0.207734763
18.1	0	0.00105179	-0.227401572	-0.208630954
18.2	0	0.001047996	-0.228304857	-0.209524855
18.3	0	0.001044311	-0.229205864	-0.210416481
18.4	0	0.001040732	-0.230104606	-0.211305843

18.5	0	0.00103726	-0.231001098	-0.212192956
18.6	0	0.001033893	-0.231895351	-0.213077832
18.7	0	0.001030631	-0.232787379	-0.213960483
18.8	0	0.001027474	-0.233677194	-0.214840923
18.9	0	0.00102442	-0.234564809	-0.215719164
19	0	0.001021469	-0.235450236	-0.216595218
19.1	0	0.00101862	-0.236333487	-0.217469098
19.2	0	0.001015872	-0.237214575	-0.218340816
19.3	0	0.001013226	-0.238093511	-0.219210384
19.4	0	0.00101068	-0.238970308	-0.220077814
19.5	0	0.001008233	-0.239844978	-0.220943117
19.6	0	0.001005886	-0.240717532	-0.221806306
19.7	0	0.001003637	-0.241587982	-0.222667392
19.8	0	0.001001485	-0.242456339	-0.223526387
19.9	0	0.000999431	-0.243322615	-0.224383303
20	0	0.000997474	-0.244186822	-0.225238149

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 100 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.005596475	0.000995734	0.018050315
0.1	0	0.005517683	-0.000974767	0.016089317
0.2	0	0.005440904	-0.002925571	0.014148014
0.3	0	0.005366022	-0.004857413	0.012225673
0.4	0	0.005292936	-0.006770972	0.010321616
0.5	0	0.005221553	-0.008666876	0.008435213
0.6	0	0.005151789	-0.01054571	0.006565879
0.7	0	0.005083566	-0.012408018	0.00471307
0.8	0	0.005016814	-0.014254312	0.002876275
0.9	0	0.004951469	-0.016085068	0.001055017

1	0	0.004887471	-0.017900737	-0.000751154
1.1	0	0.004824766	-0.019701742	-0.002542662
1.2	0	0.004763301	-0.021488481	-0.004319905
1.3	0	0.004703029	-0.023261333	-0.00608326
1.4	0	0.004643907	-0.025020654	-0.007833086
1.5	0	0.004585891	-0.026766785	-0.009569722
1.6	0	0.004528945	-0.028500046	-0.011293489
1.7	0	0.004473032	-0.030220746	-0.013004695
1.8	0	0.004418117	-0.031929175	-0.014703631
1.9	0	0.004364168	-0.033625613	-0.016390577
2	0	0.004311154	-0.035310326	-0.018065798
2.1	0	0.004259049	-0.036983568	-0.019729549
2.2	0	0.004207824	-0.038645583	-0.021382074
2.3	0	0.004157453	-0.040296606	-0.023023606
2.4	0	0.004107912	-0.041936858	-0.02465437
2.5	0	0.004059179	-0.043566557	-0.02627458
2.6	0	0.004011231	-0.045185908	-0.027884443
2.7	0	0.003964048	-0.046795111	-0.029484158
2.8	0	0.003917609	-0.048394357	-0.031073917
2.9	0	0.003871895	-0.04998383	-0.032653904
3	0	0.003826888	-0.051563708	-0.034224297
3.1	0	0.003782572	-0.053134164	-0.035785268
3.2	0	0.003738929	-0.054695362	-0.037336981
3.3	0	0.003695944	-0.056247462	-0.038879599
3.4	0	0.0036536	-0.057790621	-0.040413274
3.5	0	0.003611884	-0.059324986	-0.041938157
3.6	0	0.003570782	-0.060850704	-0.043454394
3.7	0	0.00353028	-0.062367914	-0.044962123
3.8	0	0.003490366	-0.063876753	-0.046461482
3.9	0	0.003451026	-0.065377352	-0.047952602
4	0	0.003412248	-0.06686984	-0.049435611
4.1	0	0.003374022	-0.068354341	-0.050910634

4.2	0	0.003336336	-0.069830975	-0.05237779
4.3	0	0.003299179	-0.071299859	-0.053837198
4.4	0	0.003262541	-0.072761108	-0.055288971
4.5	0	0.003226412	-0.074214831	-0.056733219
4.6	0	0.003190782	-0.075661138	-0.058170051
4.7	0	0.003155642	-0.077100132	-0.059599571
4.8	0	0.003120983	-0.078531915	-0.061021882
4.9	0	0.003086796	-0.079956588	-0.062437082
5	0	0.003053073	-0.081374246	-0.063845269
5.1	0	0.003019804	-0.082784984	-0.065246536
5.2	0	0.002986984	-0.084188894	-0.066640976
5.3	0	0.002954603	-0.085586066	-0.068028679
5.4	0	0.002922654	-0.086976588	-0.069409732
5.5	0	0.00289113	-0.088360544	-0.07078422
5.6	0	0.002860024	-0.089738018	-0.072152227
5.7	0	0.002829329	-0.091109091	-0.073513834
5.8	0	0.002799038	-0.092473844	-0.074869121
5.9	0	0.002769146	-0.093832353	-0.076218166
6	0	0.002739645	-0.095184696	-0.077561044
6.1	0	0.002710529	-0.096530945	-0.078897829
6.2	0	0.002681793	-0.097871173	-0.080228596
6.3	0	0.002653431	-0.099205452	-0.081553413
6.4	0	0.002625437	-0.100533852	-0.082872351
6.5	0	0.002597806	-0.101856439	-0.084185479
6.6	0	0.002570532	-0.103173282	-0.085492862
6.7	0	0.00254361	-0.104484444	-0.086794565
6.8	0	0.002517036	-0.10578999	-0.088090653
6.9	0	0.002490803	-0.107089981	-0.089381188
7	0	0.002464907	-0.108384481	-0.090666231
7.1	0	0.002439344	-0.109673548	-0.091945843
7.2	0	0.00241411	-0.110957241	-0.093220082
7.3	0	0.002389198	-0.112235619	-0.094489005

7.4	0	0.002364606	-0.113508737	-0.095752671
7.5	0	0.002340328	-0.114776652	-0.097011133
7.6	0	0.002316361	-0.116039417	-0.098264446
7.7	0	0.002292701	-0.117297086	-0.099512665
7.8	0	0.002269343	-0.118549711	-0.100755841
7.9	0	0.002246283	-0.119797344	-0.101994025
8	0	0.002223519	-0.121040036	-0.103227269
8.1	0	0.002201046	-0.122277836	-0.104455621
8.2	0	0.00217886	-0.123510792	-0.105679131
8.3	0	0.002156957	-0.124738953	-0.106897846
8.4	0	0.002135336	-0.125962365	-0.108111814
8.5	0	0.002113991	-0.127181075	-0.10932108
8.6	0	0.00209292	-0.128395128	-0.11052569
8.7	0	0.002072119	-0.129604569	-0.111725689
8.8	0	0.002051585	-0.130809441	-0.112921119
8.9	0	0.002031316	-0.132009787	-0.114112025
9	0	0.002011307	-0.133205651	-0.115298449
9.1	0	0.001991555	-0.134397073	-0.116480433
9.2	0	0.001972059	-0.135584094	-0.117658016
9.3	0	0.001952815	-0.136766756	-0.118831241
9.4	0	0.00193382	-0.137945097	-0.120000146
9.5	0	0.001915071	-0.139119156	-0.12116477
9.6	0	0.001896565	-0.140288973	-0.122325152
9.7	0	0.001878301	-0.141454584	-0.12348133
9.8	0	0.001860275	-0.142616027	-0.124633341
9.9	0	0.001842484	-0.143773339	-0.125781221
10	0	0.001824927	-0.144926555	-0.126925006
10.1	0	0.001807601	-0.146075711	-0.128064733
10.2	0	0.001790502	-0.147220843	-0.129200436
10.3	0	0.00177363	-0.148361984	-0.130332149
10.4	0	0.00175698	-0.149499169	-0.131459906
10.5	0	0.001740552	-0.150632431	-0.132583742

10.6	0	0.001724343	-0.151761802	-0.133703688
10.7	0	0.00170835	-0.152887316	-0.134819777
10.8	0	0.001692572	-0.154009004	-0.135932042
10.9	0	0.001677006	-0.155126898	-0.137040513
11	0	0.00166165	-0.156241029	-0.138145222
11.1	0	0.001646502	-0.157351427	-0.1392462
11.2	0	0.00163156	-0.158458123	-0.140343476
11.3	0	0.001616822	-0.159561146	-0.14143708
11.4	0	0.001602286	-0.160660527	-0.142527043
11.5	0	0.001587949	-0.161756293	-0.143613392
11.6	0	0.001573812	-0.162848473	-0.144696156
11.7	0	0.00155987	-0.163937096	-0.145775364
11.8	0	0.001546122	-0.165022189	-0.146851043
11.9	0	0.001532567	-0.16610378	-0.14792322
12	0	0.001519203	-0.167181896	-0.148991924
12.1	0	0.001506028	-0.168256563	-0.150057179
12.2	0	0.00149304	-0.169327808	-0.151119014
12.3	0	0.001480237	-0.170395656	-0.152177453
12.4	0	0.001467619	-0.171460134	-0.153232522
12.5	0	0.001455182	-0.172521267	-0.154284247
12.6	0	0.001442926	-0.173579079	-0.155332653
12.7	0	0.001430849	-0.174633596	-0.156377764
12.8	0	0.001418949	-0.175684841	-0.157419605
12.9	0	0.001407224	-0.17673284	-0.158458199
13	0	0.001395675	-0.177777615	-0.159493572
13.1	0	0.001384297	-0.178819189	-0.160525745
13.2	0	0.001373091	-0.179857587	-0.161554742
13.3	0	0.001362054	-0.180892831	-0.162580586
13.4	0	0.001351186	-0.181924944	-0.1636033
13.5	0	0.001340485	-0.182953948	-0.164622906
13.6	0	0.001329949	-0.183979864	-0.165639425
13.7	0	0.001319577	-0.185002716	-0.166652881

13.8	0	0.001309367	-0.186022523	-0.167663294
13.9	0	0.001299319	-0.187039309	-0.168670685
14	0	0.001289431	-0.188053093	-0.169675076
14.1	0	0.001279701	-0.189063896	-0.170676488
14.2	0	0.001270129	-0.190071739	-0.17167494
14.3	0	0.001260713	-0.191076643	-0.172670454
14.4	0	0.001251452	-0.192078627	-0.173663049
14.5	0	0.001242344	-0.193077711	-0.174652745
14.6	0	0.001233389	-0.194073914	-0.175639562
14.7	0	0.001224584	-0.195067257	-0.176623519
14.8	0	0.00121593	-0.196057758	-0.177604635
14.9	0	0.001207424	-0.197045436	-0.178582929
15	0	0.001199066	-0.19803031	-0.17955842
15.1	0	0.001190854	-0.199012398	-0.180531127
15.2	0	0.001182788	-0.19999172	-0.181501067
15.3	0	0.001174865	-0.200968292	-0.18246826
15.4	0	0.001167086	-0.201942133	-0.183432722
15.5	0	0.001159449	-0.20291326	-0.184394472
15.6	0	0.001151952	-0.203881692	-0.185353527
15.7	0	0.001144596	-0.204847445	-0.186309904
15.8	0	0.001137378	-0.205810536	-0.187263621
15.9	0	0.001130298	-0.206770983	-0.188214694
16	0	0.001123355	-0.207728802	-0.189163141
16.1	0	0.001116548	-0.20868401	-0.190108978
16.2	0	0.001109875	-0.209636624	-0.191052221
16.3	0	0.001103336	-0.210586659	-0.191992887
16.4	0	0.001096929	-0.211534132	-0.192930991
16.5	0	0.001090655	-0.212479059	-0.19386655
16.6	0	0.001084511	-0.213421455	-0.19479958
16.7	0	0.001078497	-0.214361336	-0.195730096
16.8	0	0.001072612	-0.215298717	-0.196658114
16.9	0	0.001066856	-0.216233615	-0.197583648

17	0	0.001061226	-0.217166043	-0.198506714
17.1	0	0.001055723	-0.218096017	-0.199427327
17.2	0	0.001050345	-0.219023552	-0.200345502
17.3	0	0.001045091	-0.219948662	-0.201261254
17.4	0	0.001039961	-0.220871362	-0.202174596
17.5	0	0.001034954	-0.221791667	-0.203085544
17.6	0	0.001030069	-0.22270959	-0.203994112
17.7	0	0.001025305	-0.223625146	-0.204900313
17.8	0	0.001020661	-0.224538349	-0.205804162
17.9	0	0.001016137	-0.225449212	-0.206705673
18	0	0.001011731	-0.226357749	-0.207604859
18.1	0	0.001007443	-0.227263975	-0.208501735
18.2	0	0.001003273	-0.228167901	-0.209396312
18.3	0	0.000999218	-0.229069542	-0.210288605
18.4	0	0.000995279	-0.229968911	-0.211178627
18.5	0	0.000991455	-0.230866021	-0.212066391
18.6	0	0.000987745	-0.231760884	-0.212951909
18.7	0	0.000984148	-0.232653514	-0.213835196
18.8	0	0.000980663	-0.233543924	-0.214716263
18.9	0	0.000977291	-0.234432125	-0.215595123
19	0	0.000974029	-0.235318131	-0.216471788
19.1	0	0.000970878	-0.236201953	-0.217346271
19.2	0	0.000967836	-0.237083605	-0.218218584
19.3	0	0.000964903	-0.237963097	-0.21908874
19.4	0	0.000962079	-0.238840443	-0.219956749
19.5	0	0.000959362	-0.239715654	-0.220822625
19.6	0	0.000956752	-0.240588741	-0.221686379
19.7	0	0.000954248	-0.241459717	-0.222548022
19.8	0	0.000951849	-0.242328593	-0.223407567
19.9	0	0.000949556	-0.243195381	-0.224265024
20	0	0.000947367	-0.244060092	-0.225120406

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 200 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.006413679	0.003500911	0.020519885
0.1	0	0.006322303	0.001516052	0.018544543
0.2	0	0.006233102	-0.000448885	0.016589122
0.3	0	0.006145961	-0.002394641	0.014652881
0.4	0	0.006060774	-0.004321903	0.012735134
0.5	0	0.005977447	-0.006231307	0.010835245
0.6	0	0.005895891	-0.008123443	0.008952623
0.7	0	0.005816029	-0.009998863	0.007086716
0.8	0	0.005737786	-0.011858082	0.005237009
0.9	0	0.005661096	-0.013701586	0.003403018
1	0	0.005585895	-0.015529828	0.001584288
1.1	0	0.005512127	-0.017343235	-0.000219608
1.2	0	0.005439737	-0.019142213	-0.002009075
1.3	0	0.005368675	-0.020927142	-0.003784494
1.4	0	0.005298895	-0.022698386	-0.005546228
1.5	0	0.005230353	-0.024456286	-0.00729462
1.6	0	0.005163008	-0.02620117	-0.009029995
1.7	0	0.00509682	-0.027933347	-0.010752664
1.8	0	0.005031754	-0.029653113	-0.012462923
1.9	0	0.004967774	-0.03136075	-0.014161053
2	0	0.00490485	-0.033056527	-0.015847324
2.1	0	0.004842949	-0.034740703	-0.017521995
2.2	0	0.004782044	-0.036413523	-0.01918531
2.3	0	0.004722105	-0.038075225	-0.020837507
2.4	0	0.004663107	-0.039726034	-0.022478813
2.5	0	0.004605025	-0.041366169	-0.024109445
2.6	0	0.004547836	-0.042995839	-0.025729613

2.7	0	0.004491515	-0.044615246	-0.027339517
2.8	0	0.004436043	-0.046224582	-0.028939352
2.9	0	0.004381398	-0.047824035	-0.030529305
3	0	0.00432756	-0.049413785	-0.032109555
3.1	0	0.00427451	-0.050994005	-0.033680276
3.2	0	0.004222231	-0.052564864	-0.035241636
3.3	0	0.004170704	-0.054126523	-0.036793797
3.4	0	0.004119914	-0.055679139	-0.038336916
3.5	0	0.004069843	-0.057222863	-0.039871143
3.6	0	0.004020477	-0.058757842	-0.041396627
3.7	0	0.003971801	-0.060284219	-0.042913508
3.8	0	0.003923801	-0.06180213	-0.044421926
3.9	0	0.003876462	-0.06331171	-0.045922012
4	0	0.003829772	-0.064813088	-0.047413897
4.1	0	0.003783717	-0.06630639	-0.048897707
4.2	0	0.003738286	-0.067791738	-0.050373563
4.3	0	0.003693467	-0.06926925	-0.051841584
4.4	0	0.003649247	-0.070739041	-0.053301885
4.5	0	0.003605616	-0.072201224	-0.054754579
4.6	0	0.003562563	-0.073655908	-0.056199774
4.7	0	0.003520077	-0.075103198	-0.057637576
4.8	0	0.00347815	-0.076543199	-0.05906809
4.9	0	0.003436769	-0.077976009	-0.060491414
5	0	0.003395927	-0.079401729	-0.061907648
5.1	0	0.003355615	-0.080820452	-0.063316886
5.2	0	0.003315822	-0.082232272	-0.064719222
5.3	0	0.003276541	-0.08363728	-0.066114747
5.4	0	0.003237763	-0.085035565	-0.067503549
5.5	0	0.00319948	-0.086427212	-0.068885715
5.6	0	0.003161684	-0.087812307	-0.070261328
5.7	0	0.003124367	-0.089190931	-0.071630472
5.8	0	0.003087522	-0.090563165	-0.072993227

5.9	0	0.003051142	-0.091929088	-0.074349672
6	0	0.00301522	-0.093288776	-0.075699882
6.1	0	0.002979747	-0.094642306	-0.077043935
6.2	0	0.002944719	-0.095989749	-0.078381902
6.3	0	0.002910129	-0.097331179	-0.079713856
6.4	0	0.002875969	-0.098666665	-0.081039868
6.5	0	0.002842234	-0.099996276	-0.082360006
6.6	0	0.002808917	-0.10132008	-0.083674337
6.7	0	0.002776014	-0.102638142	-0.084982927
6.8	0	0.002743518	-0.103950527	-0.086285841
6.9	0	0.002711423	-0.105257299	-0.087583143
7	0	0.002679724	-0.106558519	-0.088874894
7.1	0	0.002648415	-0.107854249	-0.090161155
7.2	0	0.002617493	-0.109144546	-0.091441985
7.3	0	0.00258695	-0.110429471	-0.092717443
7.4	0	0.002556783	-0.111709081	-0.093987586
7.5	0	0.002526986	-0.11298343	-0.095252471
7.6	0	0.002497555	-0.114252575	-0.096512152
7.7	0	0.002468484	-0.11551657	-0.097766684
7.8	0	0.002439771	-0.116775467	-0.099016118
7.9	0	0.002411409	-0.118029319	-0.100260509
8	0	0.002383395	-0.119278177	-0.101499906
8.1	0	0.002355724	-0.12052209	-0.10273436
8.2	0	0.002328392	-0.121761109	-0.10396392
8.3	0	0.002301396	-0.122995281	-0.105188634
8.4	0	0.00227473	-0.124224654	-0.10640855
8.5	0	0.002248392	-0.125449274	-0.107623715
8.6	0	0.002222377	-0.126669189	-0.108834174
8.7	0	0.002196682	-0.127884442	-0.110039973
8.8	0	0.002171303	-0.129095078	-0.111241157
8.9	0	0.002146235	-0.130301141	-0.112437767
9	0	0.002121477	-0.131502674	-0.113629848

9.1	0	0.002097024	-0.132699718	-0.114817442
9.2	0	0.002072873	-0.133892315	-0.11600059
9.3	0	0.00204902	-0.135080506	-0.117179333
9.4	0	0.002025462	-0.136264331	-0.11835371
9.5	0	0.002002197	-0.137443829	-0.119523762
9.6	0	0.00197922	-0.13861904	-0.120689528
9.7	0	0.001956529	-0.139790002	-0.121851045
9.8	0	0.001934121	-0.140956751	-0.123008351
9.9	0	0.001911993	-0.142119326	-0.124161483
10	0	0.001890141	-0.143277763	-0.125310478
10.1	0	0.001868564	-0.144432097	-0.126455371
10.2	0	0.001847257	-0.145582364	-0.127596199
10.3	0	0.001826219	-0.146728598	-0.128732995
10.4	0	0.001805446	-0.147870835	-0.129865794
10.5	0	0.001784937	-0.149009109	-0.130994631
10.6	0	0.001764687	-0.150143451	-0.132119537
10.7	0	0.001744696	-0.151273895	-0.133240547
10.8	0	0.001724959	-0.152400473	-0.134357692
10.9	0	0.001705475	-0.153523218	-0.135471005
11	0	0.001686241	-0.154642161	-0.136580516
11.1	0	0.001667255	-0.155757332	-0.137686256
11.2	0	0.001648515	-0.156868762	-0.138788257
11.3	0	0.001630018	-0.157976482	-0.139886549
11.4	0	0.001611761	-0.159080521	-0.14098116
11.5	0	0.001593743	-0.160180907	-0.142072121
11.6	0	0.001575961	-0.161277672	-0.143159459
11.7	0	0.001558413	-0.162370841	-0.144243205
11.8	0	0.001541097	-0.163460445	-0.145323385
11.9	0	0.001524011	-0.164546509	-0.146400028
12	0	0.001507152	-0.165629063	-0.14747316
12.1	0	0.001490519	-0.166708132	-0.14854281
12.2	0	0.00147411	-0.167783744	-0.149609002

12.3	0	0.001457922	-0.168855924	-0.150671765
12.4	0	0.001441954	-0.169924699	-0.151731123
12.5	0	0.001426204	-0.170990094	-0.152787103
12.6	0	0.001410669	-0.172052134	-0.153839728
12.7	0	0.001395348	-0.173110845	-0.154889026
12.8	0	0.00138024	-0.174166251	-0.155935019
12.9	0	0.001365341	-0.175218377	-0.156977733
13	0	0.001350651	-0.176267245	-0.158017192
13.1	0	0.001336168	-0.177312881	-0.159053418
13.2	0	0.00132189	-0.178355307	-0.160086437
13.3	0	0.001307815	-0.179394547	-0.161116269
13.4	0	0.001293941	-0.180430623	-0.16214294
13.5	0	0.001280267	-0.181463558	-0.16316647
13.6	0	0.001266791	-0.182493375	-0.164186883
13.7	0	0.001253512	-0.183520095	-0.165204201
13.8	0	0.001240428	-0.18454374	-0.166218445
13.9	0	0.001227537	-0.185564331	-0.167229636
14	0	0.001214838	-0.186581891	-0.168237797
14.1	0	0.001202329	-0.187596439	-0.169242947
14.2	0	0.001190009	-0.188607997	-0.170245109
14.3	0	0.001177876	-0.189616586	-0.171244301
14.4	0	0.00116593	-0.190622224	-0.172240545
14.5	0	0.001154167	-0.191624933	-0.173233861
14.6	0	0.001142587	-0.192624732	-0.174224268
14.7	0	0.001131189	-0.193621641	-0.175211786
14.8	0	0.00111997	-0.19461568	-0.176196435
14.9	0	0.001108931	-0.195606866	-0.177178233
15	0	0.001098068	-0.196595221	-0.178157199
15.1	0	0.001087381	-0.197580761	-0.179133353
15.2	0	0.00107687	-0.198563505	-0.180106712
15.3	0	0.001066531	-0.199543473	-0.181077296
15.4	0	0.001056365	-0.200520681	-0.182045121

15.5	0	0.001046369	-0.201495148	-0.183010207
15.6	0	0.001036543	-0.202466892	-0.18397257
15.7	0	0.001026884	-0.20343593	-0.184932229
15.8	0	0.001017393	-0.20440228	-0.1858892
15.9	0	0.001008068	-0.205365958	-0.186843502
16	0	0.000998907	-0.206326982	-0.18779515
16.1	0	0.00098991	-0.207285368	-0.188744161
16.2	0	0.000981074	-0.208241133	-0.189690553
16.3	0	0.0009724	-0.209194293	-0.190634341
16.4	0	0.000963886	-0.210144865	-0.191575543
16.5	0	0.00095553	-0.211092866	-0.192514173
16.6	0	0.000947332	-0.212038309	-0.193450248
16.7	0	0.000939291	-0.212981213	-0.194383784
16.8	0	0.000931405	-0.213921591	-0.195314797
16.9	0	0.000923673	-0.21485946	-0.196243301
17	0	0.000916094	-0.215794835	-0.197169312
17.1	0	0.000908668	-0.216727731	-0.198092846
17.2	0	0.000901393	-0.217658163	-0.199013917
17.3	0	0.000894269	-0.218586146	-0.19993254
17.4	0	0.000887293	-0.219511695	-0.20084873
17.5	0	0.000880465	-0.220434823	-0.201762501
17.6	0	0.000873785	-0.221355546	-0.202673867
17.7	0	0.000867251	-0.222273878	-0.203582844
17.8	0	0.000860862	-0.223189833	-0.204489445
17.9	0	0.000854617	-0.224103424	-0.205393684
18	0	0.000848515	-0.225014666	-0.206295575
18.1	0	0.000842556	-0.225923573	-0.207195132
18.2	0	0.000836738	-0.226830158	-0.208092368
18.3	0	0.00083106	-0.227734434	-0.208987297
18.4	0	0.000825522	-0.228636415	-0.209879932
18.5	0	0.000820123	-0.229536115	-0.210770286
18.6	0	0.000814861	-0.230433545	-0.211658373

18.7	0	0.000809737	-0.231328719	-0.212544205
18.8	0	0.000804748	-0.232221651	-0.213427795
18.9	0	0.000799894	-0.233112351	-0.214309156
19	0	0.000795175	-0.234000835	-0.2151883
19.1	0	0.000790589	-0.234887112	-0.216065241
19.2	0	0.000786136	-0.235771197	-0.21693999
19.3	0	0.000781814	-0.236653102	-0.217812559
19.4	0	0.000777623	-0.237532837	-0.218682961
19.5	0	0.000773563	-0.238410416	-0.219551208
19.6	0	0.000769632	-0.239285851	-0.220417312
19.7	0	0.000765829	-0.240159153	-0.221281285
19.8	0	0.000762154	-0.241030334	-0.222143137
19.9	0	0.000758606	-0.241899405	-0.223002882
20	0	0.000755185	-0.242766379	-0.22386053

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 300 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.007301054	0.007478085	0.024424983
0.1	0	0.007197565	0.005478515	0.022434922
0.2	0	0.007096304	0.003499037	0.02046495
0.3	0	0.006997164	0.001538907	0.018514327
0.4	0	0.006900047	-0.000402563	0.016582364
0.5	0	0.006804863	-0.00232601	0.014668423
0.6	0	0.006711529	-0.004232026	0.012771911
0.7	0	0.006619969	-0.006121167	0.010892276
0.8	0	0.006530114	-0.007993949	0.009028998
0.9	0	0.006441898	-0.009850859	0.007181591
1	0	0.00635526	-0.011692354	0.005349599
1.1	0	0.006270146	-0.013518865	0.003532592

1.2	0	0.006186501	-0.015330797	0.001730161
1.3	0	0.006104276	-0.017128536	-0.0000580758
1.4	0	0.006023426	-0.018912445	-0.001832484
1.5	0	0.005943906	-0.02068287	-0.003593409
1.6	0	0.005865676	-0.02244014	-0.005341179
1.7	0	0.005788697	-0.024184568	-0.007076107
1.8	0	0.005712933	-0.02591645	-0.008798491
1.9	0	0.005638348	-0.027636072	-0.010508615
2	0	0.00556491	-0.029343706	-0.012206751
2.1	0	0.005492589	-0.03103961	-0.013893159
2.2	0	0.005421353	-0.032724034	-0.015568087
2.3	0	0.005351176	-0.034397217	-0.017231774
2.4	0	0.00528203	-0.036059386	-0.018884449
2.5	0	0.00521389	-0.037710763	-0.020526331
2.6	0	0.005146731	-0.039351558	-0.022157632
2.7	0	0.00508053	-0.040981974	-0.023778555
2.8	0	0.005015264	-0.042602207	-0.025389296
2.9	0	0.004950912	-0.044212445	-0.026990042
3	0	0.004887454	-0.045812871	-0.028580977
3.1	0	0.004824869	-0.047403659	-0.030162274
3.2	0	0.004763139	-0.048984979	-0.031734105
3.3	0	0.004702246	-0.050556995	-0.033296632
3.4	0	0.004642172	-0.052119865	-0.034850014
3.5	0	0.0045829	-0.053673743	-0.036394403
3.6	0	0.004524414	-0.055218775	-0.037929949
3.7	0	0.004466699	-0.056755107	-0.039456794
3.8	0	0.004409739	-0.058282876	-0.040975077
3.9	0	0.00435352	-0.059802219	-0.042484935
4	0	0.004298027	-0.061313265	-0.043986497
4.1	0	0.004243248	-0.062816142	-0.045479891
4.2	0	0.004189168	-0.064310974	-0.046965239
4.3	0	0.004135777	-0.06579788	-0.048442663

4.4	0	0.00408306	-0.067276976	-0.049912278
4.5	0	0.004031006	-0.068748376	-0.051374197
4.6	0	0.003979604	-0.070212191	-0.052828532
4.7	0	0.003928843	-0.071668526	-0.054275388
4.8	0	0.003878712	-0.073117488	-0.055714871
4.9	0	0.003829199	-0.074559177	-0.057147082
5	0	0.003780296	-0.075993692	-0.05857212
5.1	0	0.003731992	-0.07742113	-0.059990082
5.2	0	0.003684277	-0.078841586	-0.061401062
5.3	0	0.003637143	-0.08025515	-0.062805152
5.4	0	0.00359058	-0.081661914	-0.064202441
5.5	0	0.003544579	-0.083061963	-0.065593017
5.6	0	0.003499132	-0.084455383	-0.066976965
5.7	0	0.00345423	-0.085842258	-0.068354368
5.8	0	0.003409866	-0.087222669	-0.069725308
5.9	0	0.00336603	-0.088596696	-0.071089865
6	0	0.003322717	-0.089964416	-0.072448116
6.1	0	0.003279918	-0.091325905	-0.073800136
6.2	0	0.003237625	-0.092681238	-0.075146001
6.3	0	0.003195832	-0.094030487	-0.076485784
6.4	0	0.003154532	-0.095373724	-0.077819554
6.5	0	0.003113718	-0.096711018	-0.079147383
6.6	0	0.003073383	-0.098042437	-0.080469337
6.7	0	0.003033521	-0.099368048	-0.081785485
6.8	0	0.002994126	-0.100687916	-0.08309589
6.9	0	0.00295519	-0.102002106	-0.084400618
7	0	0.002916709	-0.103310679	-0.08569973
7.1	0	0.002878677	-0.104613698	-0.086993289
7.2	0	0.002841088	-0.105911223	-0.088281354
7.3	0	0.002803935	-0.107203313	-0.089563985
7.4	0	0.002767214	-0.108490025	-0.09084124
7.5	0	0.002730919	-0.109771417	-0.092113175

7.6	0	0.002695045	-0.111047544	-0.093379846
7.7	0	0.002659587	-0.11231846	-0.094641307
7.8	0	0.002624539	-0.113584221	-0.095897613
7.9	0	0.002589898	-0.114844877	-0.097148816
8	0	0.002555657	-0.116100482	-0.098394968
8.1	0	0.002521813	-0.117351085	-0.099636119
8.2	0	0.00248836	-0.118596736	-0.10087232
8.3	0	0.002455294	-0.119837485	-0.102103619
8.4	0	0.002422611	-0.12107338	-0.103330064
8.5	0	0.002390306	-0.122304467	-0.104551704
8.6	0	0.002358375	-0.123530793	-0.105768583
8.7	0	0.002326814	-0.124752405	-0.106980748
8.8	0	0.002295619	-0.125969346	-0.108188243
8.9	0	0.002264785	-0.127181661	-0.109391114
9	0	0.002234309	-0.128389393	-0.110589402
9.1	0	0.002204187	-0.129592585	-0.111783151
9.2	0	0.002174415	-0.130791278	-0.112972403
9.3	0	0.002144989	-0.131985515	-0.114157199
9.4	0	0.002115906	-0.133175336	-0.11533758
9.5	0	0.002087161	-0.13436078	-0.116513584
9.6	0	0.002058753	-0.135541886	-0.117685253
9.7	0	0.002030676	-0.136718695	-0.118852624
9.8	0	0.002002928	-0.137891243	-0.120015736
9.9	0	0.001975505	-0.139059568	-0.121174626
10	0	0.001948404	-0.140223707	-0.122329331
10.1	0	0.001921622	-0.141383697	-0.123479887
10.2	0	0.001895156	-0.142539572	-0.12462633
10.3	0	0.001869002	-0.143691369	-0.125768696
10.4	0	0.001843157	-0.144839123	-0.126907019
10.5	0	0.001817619	-0.145982866	-0.128041333
10.6	0	0.001792384	-0.147122634	-0.129171672
10.7	0	0.001767449	-0.148258458	-0.130298069

10.8	0	0.001742813	-0.149390373	-0.131420557
10.9	0	0.001718471	-0.15051841	-0.132539169
11	0	0.001694421	-0.151642601	-0.133653935
11.1	0	0.00167066	-0.152762978	-0.134764888
11.2	0	0.001647186	-0.15387957	-0.135872058
11.3	0	0.001623996	-0.15499241	-0.136975476
11.4	0	0.001601087	-0.156101526	-0.138075171
11.5	0	0.001578457	-0.157206948	-0.139171174
11.6	0	0.001556104	-0.158308706	-0.140263513
11.7	0	0.001534024	-0.159406829	-0.141352218
11.8	0	0.001512215	-0.160501344	-0.142437317
11.9	0	0.001490675	-0.16159228	-0.143518838
12	0	0.001469402	-0.162679665	-0.144596808
12.1	0	0.001448393	-0.163763526	-0.145671255
12.2	0	0.001427646	-0.16484389	-0.146742206
12.3	0	0.001407159	-0.165920782	-0.147809687
12.4	0	0.001386929	-0.166994231	-0.148873725
12.5	0	0.001366955	-0.168064261	-0.149934346
12.6	0	0.001347233	-0.169130898	-0.150991574
12.7	0	0.001327763	-0.170194168	-0.152045437
12.8	0	0.001308541	-0.171254094	-0.153095957
12.9	0	0.001289566	-0.172310703	-0.15414316
13	0	0.001270835	-0.173364018	-0.155187071
13.1	0	0.001252347	-0.174414063	-0.156227713
13.2	0	0.0012341	-0.175460862	-0.157265109
13.3	0	0.001216092	-0.176504438	-0.158299284
13.4	0	0.001198321	-0.177544814	-0.159330261
13.5	0	0.001180784	-0.178582014	-0.160358062
13.6	0	0.00116348	-0.179616059	-0.161382709
13.7	0	0.001146408	-0.180646973	-0.162404226
13.8	0	0.001129564	-0.181674777	-0.163422634
13.9	0	0.001112949	-0.182699492	-0.164437955

14	0	0.001096559	-0.183721141	-0.16545021
14.1	0	0.001080393	-0.184739745	-0.166459421
14.2	0	0.001064449	-0.185755323	-0.167465608
14.3	0	0.001048725	-0.186767899	-0.168468793
14.4	0	0.001033221	-0.187777491	-0.169468996
14.5	0	0.001017934	-0.188784121	-0.170466238
14.6	0	0.001002862	-0.189787807	-0.171460537
14.7	0	0.000988004	-0.190788571	-0.172451915
14.8	0	0.000973358	-0.191786431	-0.17344039
14.9	0	0.000958923	-0.192781407	-0.174425983
15	0	0.000944697	-0.193773519	-0.175408711
15.1	0	0.000930679	-0.194762784	-0.176388595
15.2	0	0.000916867	-0.195749222	-0.177365653
15.3	0	0.000903259	-0.196732852	-0.178339903
15.4	0	0.000889854	-0.197713691	-0.179311364
15.5	0	0.000876651	-0.198691758	-0.180280054
15.6	0	0.000863648	-0.199667071	-0.181245991
15.7	0	0.000850844	-0.200639648	-0.182209193
15.8	0	0.000838237	-0.201609505	-0.183169676
15.9	0	0.000825826	-0.20257666	-0.184127459
16	0	0.000813609	-0.203541132	-0.185082559
16.1	0	0.000801586	-0.204502935	-0.186034992
16.2	0	0.000789754	-0.205462088	-0.186984776
16.3	0	0.000778113	-0.206418607	-0.187931927
16.4	0	0.00076666	-0.207372509	-0.188876461
16.5	0	0.000755396	-0.208323809	-0.189818396
16.6	0	0.000744318	-0.209272524	-0.190757746
16.7	0	0.000733426	-0.210218669	-0.191694528
16.8	0	0.000722717	-0.211162262	-0.192628758
16.9	0	0.000712191	-0.212103316	-0.193560452
17	0	0.000701847	-0.213041849	-0.194489624
17.1	0	0.000691683	-0.213977874	-0.195416291

17.2	0	0.000681698	-0.214911408	-0.196340467
17.3	0	0.000671891	-0.215842464	-0.197262167
17.4	0	0.000662261	-0.216771059	-0.198181406
17.5	0	0.000652806	-0.217697207	-0.1990982
17.6	0	0.000643526	-0.218620921	-0.200012561
17.7	0	0.000634419	-0.219542218	-0.200924506
17.8	0	0.000625484	-0.220461111	-0.201834049
17.9	0	0.00061672	-0.221377614	-0.202741202
18	0	0.000608126	-0.222291741	-0.203645981
18.1	0	0.000599701	-0.223203507	-0.204548399
18.2	0	0.000591444	-0.224112924	-0.205448471
18.3	0	0.000583353	-0.225020007	-0.206346209
18.4	0	0.000575428	-0.225924768	-0.207241627
18.5	0	0.000567668	-0.226827222	-0.208134739
18.6	0	0.000560071	-0.227727382	-0.209025557
18.7	0	0.000552637	-0.22862526	-0.209914096
18.8	0	0.000545364	-0.22952087	-0.210800367
18.9	0	0.000538252	-0.230414225	-0.211684384
19	0	0.000531299	-0.231305336	-0.212566159
19.1	0	0.000524505	-0.232194218	-0.213445706
19.2	0	0.000517869	-0.233080882	-0.214323036
19.3	0	0.000511389	-0.233965341	-0.215198162
19.4	0	0.000505064	-0.234847606	-0.216071096
19.5	0	0.000498895	-0.235727692	-0.216941851
19.6	0	0.000492879	-0.236605608	-0.217810439
19.7	0	0.000487017	-0.237481368	-0.218676871
19.8	0	0.000481306	-0.238354983	-0.219541159
19.9	0	0.000475746	-0.239226464	-0.220403315
20	0	0.000470336	-0.240095825	-0.221263351

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 400 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.008220049	0.01211015	0.028966304
0.1	0	0.00810431	0.01009675	0.026962397
0.2	0	0.00799079	0.008103545	0.024978684
0.3	0	0.007879394	0.006129795	0.023014426
0.4	0	0.007770038	0.00417482	0.021068942
0.5	0	0.007662642	0.002237984	0.019141598
0.6	0	0.007557133	0.000318698	0.017231802
0.7	0	0.007453442	-0.001583591	0.015339003
0.8	0	0.007351506	-0.003469398	0.013462685
0.9	0	0.007251265	-0.00533921	0.011602362
1	0	0.007152664	-0.007193482	0.009757578
1.1	0	0.007055651	-0.009032645	0.007927903
1.2	0	0.006960175	-0.010857106	0.006112929
1.3	0	0.006866191	-0.012667248	0.004312273
1.4	0	0.006773654	-0.014463438	0.00252557
1.5	0	0.006682524	-0.016246021	0.000752472
1.6	0	0.006592761	-0.018015327	-0.001007349
1.7	0	0.006504328	-0.019771669	-0.002754206
1.8	0	0.006417189	-0.021515345	-0.004488399
1.9	0	0.00633131	-0.023246643	-0.006210213
2	0	0.006246661	-0.024965833	-0.00791992
2.1	0	0.006163209	-0.026673177	-0.009617783
2.2	0	0.006080926	-0.028368926	-0.011304049
2.3	0	0.005999785	-0.030053318	-0.012978961
2.4	0	0.005919757	-0.031726584	-0.014642747
2.5	0	0.005840819	-0.033388945	-0.016295628
2.6	0	0.005762945	-0.035040614	-0.017937818

2.7	0	0.005686112	-0.036681794	-0.019569519
2.8	0	0.005610297	-0.038312683	-0.02119093
2.9	0	0.005535479	-0.03993347	-0.022802241
3	0	0.005461637	-0.041544339	-0.024403633
3.1	0	0.005388751	-0.043145466	-0.025995284
3.2	0	0.005316802	-0.044737022	-0.027577365
3.3	0	0.005245771	-0.046319172	-0.02915004
3.4	0	0.005175639	-0.047892075	-0.030713469
3.5	0	0.005106391	-0.049455886	-0.032267806
3.6	0	0.005038009	-0.051010753	-0.033813201
3.7	0	0.004970477	-0.052556823	-0.035349798
3.8	0	0.004903779	-0.054094234	-0.036877738
3.9	0	0.004837901	-0.055623124	-0.038397157
4	0	0.004772828	-0.057143623	-0.039908187
4.1	0	0.004708545	-0.058655861	-0.041410955
4.2	0	0.00464504	-0.060159962	-0.042905587
4.3	0	0.004582298	-0.061656046	-0.044392204
4.4	0	0.004520307	-0.063144232	-0.045870922
4.5	0	0.004459055	-0.064624633	-0.047341857
4.6	0	0.004398529	-0.066097361	-0.048805119
4.7	0	0.004338717	-0.067562524	-0.050260817
4.8	0	0.004279609	-0.069020228	-0.051709056
4.9	0	0.004221194	-0.070470574	-0.053149939
5	0	0.004163459	-0.071913664	-0.054583566
5.1	0	0.004106396	-0.073349595	-0.056010034
5.2	0	0.004049993	-0.074778461	-0.057429438
5.3	0	0.003994241	-0.076200356	-0.058841872
5.4	0	0.00393913	-0.077615369	-0.060247426
5.5	0	0.003884651	-0.07902359	-0.061646187
5.6	0	0.003830795	-0.080425104	-0.063038243
5.7	0	0.003777553	-0.081819996	-0.064423677
5.8	0	0.003724915	-0.083208348	-0.065802571

5.9	0	0.003672874	-0.08459024	-0.067175007
6	0	0.003621422	-0.085965751	-0.068541062
6.1	0	0.003570549	-0.087334958	-0.069900814
6.2	0	0.00352025	-0.088697935	-0.071254337
6.3	0	0.003470514	-0.090054757	-0.072601705
6.4	0	0.003421337	-0.091405494	-0.07394299
6.5	0	0.003372708	-0.092750218	-0.075278262
6.6	0	0.003324623	-0.094088998	-0.076607591
6.7	0	0.003277074	-0.0954219	-0.077931042
6.8	0	0.003230053	-0.096748991	-0.079248684
6.9	0	0.003183555	-0.098070336	-0.08056058
7	0	0.003137572	-0.099385997	-0.081866794
7.1	0	0.003092099	-0.100696038	-0.083167388
7.2	0	0.003047128	-0.102000519	-0.084462422
7.3	0	0.003002655	-0.1032995	-0.085751957
7.4	0	0.002958673	-0.104593038	-0.087036051
7.5	0	0.002915176	-0.105881193	-0.088314762
7.6	0	0.002872158	-0.10716402	-0.089588146
7.7	0	0.002829614	-0.108441574	-0.090856258
7.8	0	0.002787538	-0.10971391	-0.092119152
7.9	0	0.002745925	-0.11098108	-0.093376882
8	0	0.002704769	-0.112243138	-0.0946295
8.1	0	0.002664066	-0.113500134	-0.095877057
8.2	0	0.002623811	-0.114752119	-0.097119604
8.3	0	0.002583998	-0.115999143	-0.098357191
8.4	0	0.002544622	-0.117241254	-0.099589865
8.5	0	0.002505679	-0.1184785	-0.100817676
8.6	0	0.002467164	-0.119710927	-0.102040669
8.7	0	0.002429072	-0.120938583	-0.10325889
8.8	0	0.002391399	-0.122161512	-0.104472386
8.9	0	0.00235414	-0.123379759	-0.105681202
9	0	0.002317292	-0.124593368	-0.106885379

9.1	0	0.002280849	-0.125802383	-0.108084963
9.2	0	0.002244808	-0.127006844	-0.109279995
9.3	0	0.002209165	-0.128206795	-0.110470518
9.4	0	0.002173915	-0.129402276	-0.111656571
9.5	0	0.002139054	-0.130593329	-0.112838196
9.6	0	0.002104579	-0.131779991	-0.114015433
9.7	0	0.002070485	-0.132962303	-0.11518832
9.8	0	0.002036769	-0.134140303	-0.116356896
9.9	0	0.002003428	-0.13531403	-0.117521199
10	0	0.001970457	-0.136483519	-0.118681266
10.1	0	0.001937853	-0.13764881	-0.119837134
10.2	0	0.001905612	-0.138809936	-0.12098884
10.3	0	0.001873732	-0.139966935	-0.122136419
10.4	0	0.001842208	-0.14111984	-0.123279906
10.5	0	0.001811037	-0.142268688	-0.124419336
10.6	0	0.001780216	-0.143413512	-0.125554743
10.7	0	0.001749742	-0.144554345	-0.12668616
10.8	0	0.001719611	-0.145691221	-0.12781362
10.9	0	0.00168982	-0.146824172	-0.128937157
11	0	0.001660367	-0.14795323	-0.130056803
11.1	0	0.001631247	-0.149078428	-0.131172588
11.2	0	0.001602459	-0.150199796	-0.132284545
11.3	0	0.001573999	-0.151317366	-0.133392704
11.4	0	0.001545865	-0.152431167	-0.134497096
11.5	0	0.001518053	-0.15354123	-0.13559775
11.6	0	0.00149056	-0.154647585	-0.136694697
11.7	0	0.001463384	-0.15575026	-0.137787965
11.8	0	0.001436522	-0.156849284	-0.138877583
11.9	0	0.001409972	-0.157944685	-0.13996358
12	0	0.00138373	-0.159036492	-0.141045983
12.1	0	0.001357795	-0.160124733	-0.142124821
12.2	0	0.001332163	-0.161209433	-0.14320012

12.3	0	0.001306832	-0.162290622	-0.144271907
12.4	0	0.001281799	-0.163368324	-0.145340209
12.5	0	0.001257062	-0.164442566	-0.146405053
12.6	0	0.001232619	-0.165513375	-0.147466463
12.7	0	0.001208467	-0.166580775	-0.148524466
12.8	0	0.001184604	-0.167644792	-0.149579087
12.9	0	0.001161028	-0.16870545	-0.150630351
13	0	0.001137735	-0.169762775	-0.151678281
13.1	0	0.001114724	-0.170816791	-0.152722904
13.2	0	0.001091993	-0.171867521	-0.153764242
13.3	0	0.00106954	-0.17291499	-0.15480232
13.4	0	0.001047361	-0.17395922	-0.15583716
13.5	0	0.001025456	-0.175000235	-0.156868786
13.6	0	0.001003822	-0.176038057	-0.15789722
13.7	0	0.000982456	-0.17707271	-0.158922486
13.8	0	0.000961357	-0.178104216	-0.159944605
13.9	0	0.000940523	-0.179132596	-0.1609636
14	0	0.000919952	-0.180157872	-0.161979492
14.1	0	0.000899642	-0.181180066	-0.162992303
14.2	0	0.00087959	-0.182199199	-0.164002054
14.3	0	0.000859795	-0.183215292	-0.165008766
14.4	0	0.000840255	-0.184228365	-0.166012459
14.5	0	0.000820968	-0.185238441	-0.167013156
14.6	0	0.000801933	-0.186245537	-0.168010875
14.7	0	0.000783146	-0.187249676	-0.169005636
14.8	0	0.000764607	-0.188250876	-0.16999746
14.9	0	0.000746314	-0.189249157	-0.170986367
15	0	0.000728265	-0.190244539	-0.171972375
15.1	0	0.000710458	-0.19123704	-0.172955503
15.2	0	0.000692891	-0.192226681	-0.173935772
15.3	0	0.000675564	-0.193213478	-0.174913199
15.4	0	0.000658473	-0.194197452	-0.175887803

15.5	0	0.000641617	-0.19517862	-0.176859602
15.6	0	0.000624996	-0.196157	-0.177828615
15.7	0	0.000608606	-0.197132611	-0.178794859
15.8	0	0.000592447	-0.19810547	-0.179758353
15.9	0	0.000576517	-0.199075595	-0.180719113
16	0	0.000560814	-0.200043003	-0.181677158
16.1	0	0.000545337	-0.201007711	-0.182632504
16.2	0	0.000530084	-0.201969737	-0.183585168
16.3	0	0.000515054	-0.202929096	-0.184535168
16.4	0	0.000500245	-0.203885807	-0.18548252
16.5	0	0.000485656	-0.204839885	-0.18642724
16.6	0	0.000471285	-0.205791347	-0.187369345
16.7	0	0.000457131	-0.206740208	-0.18830885
16.8	0	0.000443192	-0.207686486	-0.189245773
16.9	0	0.000429467	-0.208630194	-0.190180128
17	0	0.000415955	-0.209571351	-0.191111932
17.1	0	0.000402654	-0.21050997	-0.192041199
17.2	0	0.000389562	-0.211446067	-0.192967946
17.3	0	0.000376679	-0.212379657	-0.193892187
17.4	0	0.000364004	-0.213310756	-0.194813938
17.5	0	0.000351533	-0.214239379	-0.195733213
17.6	0	0.000339268	-0.215165539	-0.196650028
17.7	0	0.000327205	-0.216089252	-0.197564396
17.8	0	0.000315344	-0.217010532	-0.198476332
17.9	0	0.000303684	-0.217929394	-0.199385851
18	0	0.000292223	-0.218845851	-0.200292967
18.1	0	0.00028096	-0.219759917	-0.201197693
18.2	0	0.000269894	-0.220671608	-0.202100044
18.3	0	0.000259024	-0.221580936	-0.203000034
18.4	0	0.000248348	-0.222487915	-0.203897675
18.5	0	0.000237865	-0.223392558	-0.204792983
18.6	0	0.000227574	-0.224294879	-0.205685969

18.7	0	0.000217474	-0.225194892	-0.206576648
18.8	0	0.000207564	-0.226092609	-0.207465032
18.9	0	0.000197842	-0.226988043	-0.208351135
19	0	0.000188308	-0.227881208	-0.209234969
19.1	0	0.00017896	-0.228772115	-0.210116547
19.2	0	0.000169797	-0.229660779	-0.210995883
19.3	0	0.000160818	-0.23054721	-0.211872987
19.4	0	0.000152022	-0.231431422	-0.212747874
19.5	0	0.000143408	-0.232313428	-0.213620554
19.6	0	0.000134975	-0.233193238	-0.214491041
19.7	0	0.000126721	-0.234070866	-0.215359347
19.8	0	0.000118647	-0.234946324	-0.216225483
19.9	0	0.00011075	-0.235819622	-0.217089461
20	0	0.000103029	-0.236690774	-0.217951294

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 500 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.009194329	0.016953686	0.033695495
0.1	0	0.009066246	0.014927665	0.031678983
0.2	0	0.00894032	0.012921875	0.029682702
0.3	0	0.008816478	0.010935592	0.027705927
0.4	0	0.008694651	0.008968142	0.025747985
0.5	0	0.008574775	0.0070189	0.023808251
0.6	0	0.008456788	0.005087283	0.02188614
0.7	0	0.008340633	0.003172744	0.019981108
0.8	0	0.008226256	0.001274772	0.018092642
0.9	0	0.008113605	-0.000607115	0.016220261
1	0	0.008002632	-0.00247337	0.014363512
1.1	0	0.007893289	-0.00432442	0.012521966

1.2	0	0.007785533	-0.00616067	0.01069522
1.3	0	0.007679323	-0.007982504	0.008882891
1.4	0	0.007574618	-0.009790283	0.007084615
1.5	0	0.007471379	-0.011584355	0.005300046
1.6	0	0.007369572	-0.013365047	0.003528857
1.7	0	0.007269161	-0.015132672	0.001770734
1.8	0	0.007170113	-0.016887529	0.0000253781
1.9	0	0.007072396	-0.018629903	-0.001707495
2	0	0.00697598	-0.020360067	-0.003428158
2.1	0	0.006880835	-0.022078282	-0.005136874
2.2	0	0.006786935	-0.023784799	-0.00683389
2.3	0	0.006694251	-0.025479856	-0.008519449
2.4	0	0.006602758	-0.027163686	-0.01019378
2.5	0	0.006512431	-0.028836508	-0.011857105
2.6	0	0.006423247	-0.030498537	-0.013509637
2.7	0	0.006335182	-0.032149978	-0.01515158
2.8	0	0.006248213	-0.033791027	-0.016783133
2.9	0	0.006162321	-0.035421876	-0.018404486
3	0	0.006077483	-0.037042708	-0.020015823
3.1	0	0.005993681	-0.038653701	-0.021617321
3.2	0	0.005910894	-0.040255025	-0.023209152
3.3	0	0.005829105	-0.041846848	-0.024791481
3.4	0	0.005748294	-0.043429328	-0.026364469
3.5	0	0.005668445	-0.045002622	-0.02792827
3.6	0	0.005589541	-0.046566879	-0.029483036
3.7	0	0.005511565	-0.048122246	-0.031028911
3.8	0	0.005434502	-0.049668862	-0.032566037
3.9	0	0.005358337	-0.051206865	-0.03409455
4	0	0.005283053	-0.052736389	-0.035614584
4.1	0	0.005208638	-0.054257562	-0.037126268
4.2	0	0.005135076	-0.055770508	-0.038629727
4.3	0	0.005062355	-0.057275351	-0.040125082

4.4	0	0.00499046	-0.058772209	-0.041612453
4.5	0	0.00491938	-0.060261196	-0.043091954
4.6	0	0.004849101	-0.061742425	-0.044563697
4.7	0	0.004779611	-0.063216004	-0.046027792
4.8	0	0.004710899	-0.064682041	-0.047484345
4.9	0	0.004642953	-0.066140638	-0.048933458
5	0	0.004575762	-0.067591896	-0.050375234
5.1	0	0.004509314	-0.069035914	-0.05180977
5.2	0	0.0044436	-0.070472788	-0.053237162
5.3	0	0.004378608	-0.071902611	-0.054657503
5.4	0	0.004314329	-0.073325473	-0.056070886
5.5	0	0.004250753	-0.074741466	-0.057477399
5.6	0	0.00418787	-0.076150674	-0.058877128
5.7	0	0.004125671	-0.077553184	-0.06027016
5.8	0	0.004064146	-0.078949078	-0.061656577
5.9	0	0.004003287	-0.080338437	-0.063036459
6	0	0.003943084	-0.081721341	-0.064409887
6.1	0	0.00388353	-0.083097867	-0.065776938
6.2	0	0.003824615	-0.084468091	-0.067137688
6.3	0	0.003766333	-0.085832088	-0.06849221
6.4	0	0.003708674	-0.087189928	-0.069840578
6.5	0	0.003651631	-0.088541685	-0.071182862
6.6	0	0.003595196	-0.089887427	-0.072519133
6.7	0	0.003539362	-0.091227223	-0.073849457
6.8	0	0.003484122	-0.092561138	-0.075173903
6.9	0	0.003429468	-0.093889239	-0.076492534
7	0	0.003375393	-0.09521159	-0.077805417
7.1	0	0.003321891	-0.096528253	-0.079112611
7.2	0	0.003268955	-0.09783929	-0.080414181
7.3	0	0.003216578	-0.099144761	-0.081710186
7.4	0	0.003164754	-0.100444725	-0.083000685
7.5	0	0.003113476	-0.101739241	-0.084285735

7.6	0	0.003062738	-0.103028365	-0.085565395
7.7	0	0.003012535	-0.104312153	-0.08683972
7.8	0	0.00296286	-0.10559066	-0.088108765
7.9	0	0.002913707	-0.10686394	-0.089372583
8	0	0.002865071	-0.108132045	-0.090631228
8.1	0	0.002816946	-0.109395028	-0.091884751
8.2	0	0.002769326	-0.11065294	-0.093133204
8.3	0	0.002722207	-0.11190583	-0.094376635
8.4	0	0.002675583	-0.113153748	-0.095615096
8.5	0	0.002629449	-0.114396742	-0.096848633
8.6	0	0.002583798	-0.115634859	-0.098077294
8.7	0	0.002538628	-0.116868147	-0.099301127
8.8	0	0.002493932	-0.118096651	-0.100520177
8.9	0	0.002449706	-0.119320416	-0.101734488
9	0	0.002405945	-0.120539487	-0.102944106
9.1	0	0.002362644	-0.121753906	-0.104149074
9.2	0	0.0023198	-0.122963718	-0.105349435
9.3	0	0.002277406	-0.124168964	-0.106545231
9.4	0	0.002235459	-0.125369687	-0.107736504
9.5	0	0.002193955	-0.126565926	-0.108923295
9.6	0	0.002152889	-0.127757721	-0.110105643
9.7	0	0.002112257	-0.128945113	-0.111283589
9.8	0	0.002072054	-0.130128141	-0.112457171
9.9	0	0.002032278	-0.131306843	-0.113626427
10	0	0.001992923	-0.132481256	-0.114791397
10.1	0	0.001953986	-0.133651418	-0.115952116
10.2	0	0.001915463	-0.134817365	-0.117108621
10.3	0	0.00187735	-0.135979134	-0.118260949
10.4	0	0.001839644	-0.13713676	-0.119409134
10.5	0	0.00180234	-0.138290279	-0.120553213
10.6	0	0.001765435	-0.139439723	-0.121693219
10.7	0	0.001728926	-0.140585129	-0.122829186

10.8	0	0.001692808	-0.141726528	-0.123961149
10.9	0	0.001657079	-0.142863955	-0.12508914
11	0	0.001621735	-0.143997441	-0.126213191
11.1	0	0.001586772	-0.145127019	-0.127333335
11.2	0	0.001552188	-0.14625272	-0.128449603
11.3	0	0.001517979	-0.147374576	-0.129562027
11.4	0	0.001484142	-0.148492617	-0.130670637
11.5	0	0.001450674	-0.149606874	-0.131775463
11.6	0	0.001417571	-0.150717377	-0.132876536
11.7	0	0.00138483	-0.151824154	-0.133973886
11.8	0	0.001352449	-0.152927236	-0.13506754
11.9	0	0.001320424	-0.154026651	-0.136157528
12	0	0.001288753	-0.155122427	-0.137243879
12.1	0	0.001257433	-0.156214592	-0.138326619
12.2	0	0.00122646	-0.157303174	-0.139405778
12.3	0	0.001195832	-0.158388201	-0.140481381
12.4	0	0.001165546	-0.159469698	-0.141553457
12.5	0	0.001135599	-0.160547692	-0.14262203
12.6	0	0.001105989	-0.161622211	-0.143687129
12.7	0	0.001076713	-0.162693279	-0.144748778
12.8	0	0.001047768	-0.163760922	-0.145807003
12.9	0	0.001019152	-0.164825165	-0.146861829
13	0	0.000990862	-0.165886033	-0.147913282
13.1	0	0.000962896	-0.166943551	-0.148961385
13.2	0	0.000935251	-0.167997743	-0.150006163
13.3	0	0.000907924	-0.169048633	-0.15104764
13.4	0	0.000880914	-0.170096245	-0.15208584
13.5	0	0.000854217	-0.171140601	-0.153120785
13.6	0	0.000827832	-0.172181727	-0.154152501
13.7	0	0.000801756	-0.173219642	-0.155181008
13.8	0	0.000775986	-0.174254372	-0.156206329
13.9	0	0.000750521	-0.175285937	-0.157228488

14	0	0.000725359	-0.17631436	-0.158247505
14.1	0	0.000700496	-0.177339663	-0.159263403
14.2	0	0.000675931	-0.178361868	-0.160276203
14.3	0	0.000651662	-0.179380994	-0.161285927
14.4	0	0.000627686	-0.180397064	-0.162292595
14.5	0	0.000604002	-0.181410098	-0.163296229
14.6	0	0.000580607	-0.182420117	-0.164296848
14.7	0	0.000557499	-0.183427141	-0.165294473
14.8	0	0.000534676	-0.18443119	-0.166289125
14.9	0	0.000512137	-0.185432285	-0.167280823
15	0	0.000489878	-0.186430443	-0.168269586
15.1	0	0.000467899	-0.187425687	-0.169255435
15.2	0	0.000446197	-0.188418033	-0.170238387
15.3	0	0.00042477	-0.189407501	-0.171218463
15.4	0	0.000403617	-0.190394111	-0.172195682
15.5	0	0.000382735	-0.19137788	-0.17317006
15.6	0	0.000362123	-0.192358827	-0.174141618
15.7	0	0.000341779	-0.19333697	-0.175110373
15.8	0	0.000321701	-0.194312327	-0.176076344
15.9	0	0.000301887	-0.195284916	-0.177039547
16	0	0.000282336	-0.196254755	-0.178
16.1	0	0.000263045	-0.19722186	-0.178957722
16.2	0	0.000244013	-0.19818625	-0.179912729
16.3	0	0.000225239	-0.199147941	-0.180865038
16.4	0	0.00020672	-0.20010695	-0.181814667
16.5	0	0.000188455	-0.201063293	-0.182761631
16.6	0	0.000170442	-0.202016988	-0.183705947
16.7	0	0.00015268	-0.202968051	-0.184647633
16.8	0	0.000135167	-0.203916497	-0.185586703
16.9	0	0.000117902	-0.204862343	-0.186523174
17	0	0.000100882	-0.205805605	-0.187457062
17.1	0	0.000084106	-0.206746298	-0.188388382

17.2	0	0.000067573	-0.207684438	-0.18931715
17.3	0	0.0000512811	-0.208620041	-0.190243382
17.4	0	0.0000352289	-0.209553121	-0.191167093
17.5	0	0.0000194148	-0.210483693	-0.192088297
17.6	0	0.0000038373	-0.211411773	-0.19300701
17.7	0	-0.000011505	-0.212337376	-0.193923246
17.8	0	-0.0000266136	-0.213260515	-0.19483702
17.9	0	-0.00004149	-0.214181206	-0.195748348
18	0	-0.0000561355	-0.215099463	-0.196657242
18.1	0	-0.0000705515	-0.2160153	-0.197563717
18.2	0	-0.0000847396	-0.216928731	-0.198467787
18.3	0	-0.000098701	-0.21783977	-0.199369467
18.4	0	-0.000112437	-0.218748431	-0.20026877
18.5	0	-0.000125949	-0.219654728	-0.20116571
18.6	0	-0.000139239	-0.220558674	-0.2020603
18.7	0	-0.000152307	-0.221460283	-0.202952554
18.8	0	-0.000165156	-0.222359567	-0.203842484
18.9	0	-0.000177785	-0.223256541	-0.204730105
19	0	-0.000190198	-0.224151216	-0.20561543
19.1	0	-0.000202394	-0.225043607	-0.206498471
19.2	0	-0.000214376	-0.225933726	-0.20737924
19.3	0	-0.000226144	-0.226821586	-0.208257752
19.4	0	-0.000237699	-0.227707198	-0.209134018
19.5	0	-0.000249044	-0.228590577	-0.210008051
19.6	0	-0.000260179	-0.229471733	-0.210879863
19.7	0	-0.000271105	-0.23035068	-0.211749467
19.8	0	-0.000281823	-0.231227429	-0.212616874
19.9	0	-0.000292335	-0.232101993	-0.213482097
20	0	-0.000302642	-0.232974383	-0.214345148

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 600 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.010242043	0.02182836	0.03845264
0.1	0	0.010100947	0.019790542	0.036424346
0.2	0	0.009961919	0.017772942	0.03441627
0.3	0	0.009824909	0.01577485	0.032427701
0.4	0	0.009689869	0.013795608	0.030457982
0.5	0	0.00955675	0.011834602	0.028506499
0.6	0	0.009425507	0.00989126	0.026572679
0.7	0	0.009296094	0.007965043	0.024655984
0.8	0	0.009168468	0.006055447	0.02275591
0.9	0	0.009042588	0.004161997	0.020871981
1	0	0.008918412	0.002284246	0.019003751
1.1	0	0.008795902	0.00042177	0.017150795
1.2	0	0.00867502	-0.001425831	0.015312714
1.3	0	0.00855573	-0.003258936	0.013489128
1.4	0	0.008437997	-0.005077907	0.011679676
1.5	0	0.008321788	-0.006883086	0.009884015
1.6	0	0.008207068	-0.0086748	0.008101819
1.7	0	0.008093809	-0.01045336	0.006332777
1.8	0	0.007981978	-0.012219063	0.004576591
1.9	0	0.007871547	-0.013972193	0.002832977
2	0	0.007762487	-0.015713023	0.001101664
2.1	0	0.007654772	-0.017441811	-0.00061761
2.2	0	0.007548375	-0.01915881	-0.002325093
2.3	0	0.007443271	-0.020864256	-0.004021025
2.4	0	0.007339434	-0.022558382	-0.005705637
2.5	0	0.007236842	-0.024241409	-0.007379149
2.6	0	0.007135471	-0.025913548	-0.009041776

2.7	0	0.007035299	-0.027575006	-0.010693722
2.8	0	0.006936304	-0.029225981	-0.012335184
2.9	0	0.006838466	-0.030866662	-0.013966354
3	0	0.006741764	-0.032497234	-0.015587415
3.1	0	0.006646178	-0.034117875	-0.017198546
3.2	0	0.00655169	-0.035728756	-0.018799917
3.3	0	0.006458281	-0.037330044	-0.020391696
3.4	0	0.006365933	-0.038921899	-0.021974043
3.5	0	0.006274629	-0.040504477	-0.023547113
3.6	0	0.006184352	-0.042077929	-0.025111058
3.7	0	0.006095085	-0.043642401	-0.026666023
3.8	0	0.006006812	-0.045198035	-0.02821215
3.9	0	0.005919518	-0.046744967	-0.029749577
4	0	0.005833187	-0.048283332	-0.031278437
4.1	0	0.005747806	-0.04981326	-0.03279886
4.2	0	0.005663359	-0.051334875	-0.034310972
4.3	0	0.005579833	-0.052848301	-0.035814895
4.4	0	0.005497214	-0.054353657	-0.037310748
4.5	0	0.005415489	-0.055851058	-0.038798648
4.6	0	0.005334645	-0.057340618	-0.040278706
4.7	0	0.005254669	-0.058822445	-0.041751032
4.8	0	0.00517555	-0.060296647	-0.043215735
4.9	0	0.005097275	-0.061763328	-0.044672916
5	0	0.005019832	-0.063222589	-0.046122679
5.1	0	0.004943211	-0.06467453	-0.047565122
5.2	0	0.0048674	-0.066119247	-0.049000342
5.3	0	0.004792388	-0.067556833	-0.050428432
5.4	0	0.004718164	-0.068987382	-0.051849486
5.5	0	0.00464472	-0.070410983	-0.053263591
5.6	0	0.004572043	-0.071827723	-0.054670837
5.7	0	0.004500125	-0.073237688	-0.056071308
5.8	0	0.004428955	-0.074640961	-0.057465089

5.9	0	0.004358525	-0.076037625	-0.058852261
6	0	0.004288825	-0.07742776	-0.060232903
6.1	0	0.004219846	-0.078811442	-0.061607095
6.2	0	0.004151579	-0.08018875	-0.062974913
6.3	0	0.004084015	-0.081559757	-0.064336431
6.4	0	0.004017147	-0.082924537	-0.065691723
6.5	0	0.003950965	-0.084283162	-0.06704086
6.6	0	0.003885462	-0.085635701	-0.068383912
6.7	0	0.003820629	-0.086982224	-0.069720949
6.8	0	0.00375646	-0.088322798	-0.071052038
6.9	0	0.003692946	-0.089657488	-0.072377243
7	0	0.00363008	-0.09098636	-0.073696631
7.1	0	0.003567853	-0.092309476	-0.075010265
7.2	0	0.003506261	-0.0936269	-0.076318205
7.3	0	0.003445295	-0.09493869	-0.077620515
7.4	0	0.003384948	-0.096244908	-0.078917252
7.5	0	0.003325213	-0.097545613	-0.080208477
7.6	0	0.003266084	-0.09884086	-0.081494246
7.7	0	0.003207555	-0.100130708	-0.082774615
7.8	0	0.003149619	-0.10141521	-0.08404964
7.9	0	0.003092269	-0.102694423	-0.085319376
8	0	0.0030355	-0.103968398	-0.086583876
8.1	0	0.002979306	-0.105237189	-0.087843192
8.2	0	0.00292368	-0.106500847	-0.089097376
8.3	0	0.002868616	-0.107759422	-0.090346477
8.4	0	0.00281411	-0.109012964	-0.091590547
8.5	0	0.002760155	-0.110261522	-0.092829634
8.6	0	0.002706746	-0.111505144	-0.094063785
8.7	0	0.002653877	-0.112743877	-0.095293049
8.8	0	0.002601543	-0.113977767	-0.09651747
8.9	0	0.002549739	-0.11520686	-0.097737096
9	0	0.002498459	-0.116431202	-0.09895197

9.1	0	0.002447699	-0.117650835	-0.100162137
9.2	0	0.002397453	-0.118865804	-0.101367641
9.3	0	0.002347717	-0.12007615	-0.102568523
9.4	0	0.002298485	-0.121281916	-0.103764826
9.5	0	0.002249754	-0.122483144	-0.104956591
9.6	0	0.002201518	-0.123679874	-0.106143859
9.7	0	0.002153772	-0.124872145	-0.10732667
9.8	0	0.002106513	-0.126059998	-0.108505063
9.9	0	0.002059736	-0.127243471	-0.109679077
10	0	0.002013436	-0.128422602	-0.11084875
10.1	0	0.001967609	-0.129597429	-0.11201412
10.2	0	0.00192225	-0.130767989	-0.113175224
10.3	0	0.001877356	-0.131934318	-0.114332099
10.4	0	0.001832923	-0.133096453	-0.115484779
10.5	0	0.001788946	-0.134254429	-0.116633302
10.6	0	0.001745422	-0.13540828	-0.117777701
10.7	0	0.001702346	-0.136558041	-0.118918011
10.8	0	0.001659715	-0.137703747	-0.120054266
10.9	0	0.001617524	-0.138845429	-0.121186499
11	0	0.001575771	-0.139983122	-0.122314744
11.1	0	0.001534451	-0.141116858	-0.123439032
11.2	0	0.00149356	-0.142246668	-0.124559396
11.3	0	0.001453096	-0.143372585	-0.125675867
11.4	0	0.001413054	-0.144494638	-0.126788477
11.5	0	0.001373431	-0.14561286	-0.127897255
11.6	0	0.001334224	-0.146727281	-0.129002233
11.7	0	0.001295429	-0.147837929	-0.13010344
11.8	0	0.001257042	-0.148944836	-0.131200906
11.9	0	0.001219061	-0.150048028	-0.13229466
12	0	0.001181483	-0.151147537	-0.13338473
12.1	0	0.001144303	-0.152243389	-0.134471144
12.2	0	0.001107519	-0.153335612	-0.135553931

12.3	0	0.001071129	-0.154424235	-0.136633119
12.4	0	0.001035127	-0.155509284	-0.137708734
12.5	0	0.000999512	-0.156590786	-0.138780803
12.6	0	0.000964281	-0.157668768	-0.139849352
12.7	0	0.00092943	-0.158743256	-0.140914409
12.8	0	0.000894958	-0.159814275	-0.141975998
12.9	0	0.00086086	-0.160881851	-0.143034146
13	0	0.000827133	-0.16194601	-0.144088877
13.1	0	0.000793777	-0.163006777	-0.145140216
13.2	0	0.000760786	-0.164064175	-0.146188189
13.3	0	0.000728159	-0.165118229	-0.147232818
13.4	0	0.000695893	-0.166168963	-0.148274129
13.5	0	0.000663985	-0.167216401	-0.149312144
13.6	0	0.000632432	-0.168260566	-0.150346887
13.7	0	0.000601233	-0.169301481	-0.151378382
13.8	0	0.000570384	-0.170339169	-0.152406651
13.9	0	0.000539883	-0.171373653	-0.153431717
14	0	0.000509728	-0.172404955	-0.154453602
14.1	0	0.000479915	-0.173433097	-0.155472328
14.2	0	0.000450442	-0.174458101	-0.156487916
14.3	0	0.000421308	-0.175479987	-0.157500389
14.4	0	0.000392509	-0.176498779	-0.158509768
14.5	0	0.000364044	-0.177514496	-0.159516073
14.6	0	0.000335909	-0.178527159	-0.160519326
14.7	0	0.000308103	-0.179536789	-0.161519547
14.8	0	0.000280623	-0.180543407	-0.162516756
14.9	0	0.000253468	-0.181547031	-0.163510974
15	0	0.000226634	-0.182547684	-0.16450222
15.1	0	0.00020012	-0.183545382	-0.165490514
15.2	0	0.000173924	-0.184540148	-0.166475876
15.3	0	0.000148042	-0.185531998	-0.167458324
15.4	0	0.000122474	-0.186520954	-0.168437878

15.5	0	0.0000972174	-0.187507032	-0.169414556
15.6	0	0.0000722695	-0.188490253	-0.170388377
15.7	0	0.0000476285	-0.189470633	-0.17135936
15.8	0	0.0000232924	-0.190448193	-0.172327523
15.9	0	-0.0000007406	-0.191422949	-0.173292883
16	0	-0.0000244727	-0.192394919	-0.174255459
16.1	0	-0.0000479059	-0.193364121	-0.175215268
16.2	0	-0.0000710421	-0.194330573	-0.176172327
16.3	0	-0.0000938831	-0.195294291	-0.177126655
16.4	0	-0.000116431	-0.196255293	-0.178078267
16.5	0	-0.000138687	-0.197213596	-0.179027181
16.6	0	-0.000160654	-0.198169216	-0.179973414
16.7	0	-0.000182334	-0.19912217	-0.180916982
16.8	0	-0.000203727	-0.200072474	-0.181857901
16.9	0	-0.000224837	-0.201020145	-0.182796188
17	0	-0.000245664	-0.201965199	-0.183731859
17.1	0	-0.000266211	-0.202907651	-0.18466493
17.2	0	-0.000286479	-0.203847517	-0.185595416
17.3	0	-0.00030647	-0.204784813	-0.186523333
17.4	0	-0.000326186	-0.205719554	-0.187448697
17.5	0	-0.000345628	-0.206651756	-0.188371522
17.6	0	-0.000364799	-0.207581434	-0.189291824
17.7	0	-0.000383699	-0.208508602	-0.190209618
17.8	0	-0.00040233	-0.209433275	-0.191124919
17.9	0	-0.000420695	-0.210355469	-0.192037741
18	0	-0.000438794	-0.211275197	-0.192948099
18.1	0	-0.000456629	-0.212192475	-0.193856007
18.2	0	-0.000474202	-0.213107316	-0.19476148
18.3	0	-0.000491514	-0.214019734	-0.195664531
18.4	0	-0.000508567	-0.214929744	-0.196565175
18.5	0	-0.000525363	-0.215837359	-0.197463426
18.6	0	-0.000541902	-0.216742593	-0.198359297

18.7	0	-0.000558187	-0.217645459	-0.199252802
18.8	0	-0.000574219	-0.218545972	-0.200143955
18.9	0	-0.000589999	-0.219444144	-0.201032768
19	0	-0.000605529	-0.220339989	-0.201919255
19.1	0	-0.00062081	-0.22123352	-0.202803429
19.2	0	-0.000635843	-0.22212475	-0.203685303
19.3	0	-0.000650631	-0.223013691	-0.20456489
19.4	0	-0.000665174	-0.223900357	-0.205442203
19.5	0	-0.000679475	-0.22478476	-0.206317255
19.6	0	-0.000693533	-0.225666912	-0.207190057
19.7	0	-0.000707351	-0.226546827	-0.208060622
19.8	0	-0.00072093	-0.227424515	-0.208928963
19.9	0	-0.000734271	-0.22829999	-0.209795091
20	0	-0.000747376	-0.229173264	-0.21065902

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 700 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.011353212	0.026677401	0.04317082
0.1	0	0.011198914	0.024628819	0.041131781
0.2	0	0.011046571	0.022600385	0.03911289
0.3	0	0.010896156	0.020591409	0.037113458
0.4	0	0.010747644	0.018601253	0.035132844
0.5	0	0.010601004	0.016629316	0.03317045
0.6	0	0.010456207	0.01467504	0.031225716
0.7	0	0.010313222	0.012737898	0.029298116
0.8	0	0.010172019	0.010817397	0.027387156
0.9	0	0.010032565	0.008913068	0.025492369
1	0	0.00989483	0.007024473	0.023613315
1.1	0	0.009758783	0.005151196	0.021749577

1.2	0	0.009624395	0.00329284	0.019900762
1.3	0	0.009491635	0.001449033	0.018066494
1.4	0	0.009360474	-0.000380584	0.016246417
1.5	0	0.009230884	-0.002196347	0.014440192
1.6	0	0.009102836	-0.003998581	0.012647496
1.7	0	0.008976303	-0.005787594	0.010868021
1.8	0	0.008851258	-0.007563681	0.009101472
1.9	0	0.008727675	-0.009327123	0.007347567
2	0	0.008605529	-0.01107819	0.005606036
2.1	0	0.008484795	-0.012817141	0.003876621
2.2	0	0.008365448	-0.014544225	0.002159074
2.3	0	0.008247465	-0.016259679	0.000453154
2.4	0	0.008130824	-0.017963733	-0.001241365
2.5	0	0.008015501	-0.019656608	-0.002924705
2.6	0	0.007901476	-0.021338515	-0.004597079
2.7	0	0.007788726	-0.02300966	-0.00625869
2.8	0	0.007677231	-0.024670239	-0.007909736
2.9	0	0.007566971	-0.026320442	-0.009550407
3	0	0.007457927	-0.027960454	-0.011180887
3.1	0	0.007350079	-0.029590453	-0.012801354
3.2	0	0.007243409	-0.031210609	-0.01441198
3.3	0	0.007137899	-0.032821089	-0.01601293
3.4	0	0.00703353	-0.034422053	-0.017604365
3.5	0	0.006930286	-0.036013659	-0.019186441
3.6	0	0.006828151	-0.037596055	-0.020759309
3.7	0	0.006727107	-0.039169389	-0.022323115
3.8	0	0.006627138	-0.040733803	-0.023878001
3.9	0	0.00652823	-0.042289435	-0.025424106
4	0	0.006430367	-0.043836417	-0.026961562
4.1	0	0.006333534	-0.045374881	-0.0284905
4.2	0	0.006237716	-0.046904952	-0.030011046
4.3	0	0.0061429	-0.048426753	-0.031523323

4.4	0	0.006049072	-0.049940404	-0.03302745
4.5	0	0.005956218	-0.051446021	-0.034523544
4.6	0	0.005864325	-0.052943717	-0.036011717
4.7	0	0.005773381	-0.054433602	-0.037492081
4.8	0	0.005683372	-0.055915784	-0.038964742
4.9	0	0.005594287	-0.057390367	-0.040429804
5	0	0.005506113	-0.058857453	-0.04188737
5.1	0	0.005418839	-0.060317142	-0.04333754
5.2	0	0.005332453	-0.061769531	-0.04478041
5.3	0	0.005246945	-0.063214714	-0.046216075
5.4	0	0.005162302	-0.064652784	-0.047644628
5.5	0	0.005078515	-0.066083831	-0.049066158
5.6	0	0.004995572	-0.067507943	-0.050480754
5.7	0	0.004913464	-0.068925206	-0.051888502
5.8	0	0.004832181	-0.070335705	-0.053289486
5.9	0	0.004751712	-0.071739521	-0.054683789
6	0	0.004672047	-0.073136736	-0.056071491
6.1	0	0.004593179	-0.074527427	-0.05745267
6.2	0	0.004515096	-0.075911673	-0.058827404
6.3	0	0.004437791	-0.077289547	-0.060195768
6.4	0	0.004361253	-0.078661125	-0.061557835
6.5	0	0.004285475	-0.080026477	-0.062913678
6.6	0	0.004210448	-0.081385675	-0.064263368
6.7	0	0.004136163	-0.082738788	-0.065606973
6.8	0	0.004062613	-0.084085884	-0.066944562
6.9	0	0.003989788	-0.085427029	-0.0682762
7	0	0.003917682	-0.086762289	-0.069601955
7.1	0	0.003846286	-0.088091726	-0.070921888
7.2	0	0.003775593	-0.089415405	-0.072236062
7.3	0	0.003705595	-0.090733386	-0.07354454
7.4	0	0.003636285	-0.092045729	-0.074847381
7.5	0	0.003567656	-0.093352493	-0.076144644

7.6	0	0.003499701	-0.094653738	-0.077436388
7.7	0	0.003432412	-0.095949518	-0.078722669
7.8	0	0.003365782	-0.097239891	-0.080003543
7.9	0	0.003299806	-0.098524911	-0.081279065
8	0	0.003234477	-0.099804632	-0.082549288
8.1	0	0.003169787	-0.101079107	-0.083814266
8.2	0	0.003105731	-0.102348387	-0.085074051
8.3	0	0.003042302	-0.103612524	-0.086328694
8.4	0	0.002979494	-0.104871568	-0.087578244
8.5	0	0.002917302	-0.106125569	-0.088822751
8.6	0	0.002855719	-0.107374574	-0.090062264
8.7	0	0.002794739	-0.108618631	-0.09129683
8.8	0	0.002734356	-0.109857787	-0.092526496
8.9	0	0.002674565	-0.111092088	-0.093751308
9	0	0.002615361	-0.11232158	-0.094971311
9.1	0	0.002556737	-0.113546306	-0.09618655
9.2	0	0.002498689	-0.114766311	-0.097397068
9.3	0	0.002441211	-0.115981637	-0.098602909
9.4	0	0.002384297	-0.117192328	-0.099804114
9.5	0	0.002327944	-0.118398424	-0.101000727
9.6	0	0.002272145	-0.119599968	-0.102192787
9.7	0	0.002216896	-0.120796998	-0.103380336
9.8	0	0.002162191	-0.121989556	-0.104563413
9.9	0	0.002108027	-0.12317768	-0.105742056
10	0	0.002054397	-0.124361409	-0.106916306
10.1	0	0.002001298	-0.125540781	-0.1080862
10.2	0	0.001948725	-0.126715833	-0.109251774
10.3	0	0.001896673	-0.127886602	-0.110413067
10.4	0	0.001845138	-0.129053125	-0.111570115
10.5	0	0.001794116	-0.130215437	-0.112722952
10.6	0	0.001743601	-0.131373573	-0.113871615
10.7	0	0.00169359	-0.132527569	-0.115016138

10.8	0	0.001644079	-0.133677458	-0.116156556
10.9	0	0.001595063	-0.134823274	-0.117292902
11	0	0.001546538	-0.135965051	-0.118425209
11.1	0	0.001498501	-0.137102821	-0.119553511
11.2	0	0.001450946	-0.138236617	-0.12067784
11.3	0	0.001403871	-0.139366471	-0.121798227
11.4	0	0.001357271	-0.140492413	-0.122914704
11.5	0	0.001311143	-0.141614476	-0.124027303
11.6	0	0.001265483	-0.142732689	-0.125136053
11.7	0	0.001220286	-0.143847083	-0.126240984
11.8	0	0.00117555	-0.144957688	-0.127342128
11.9	0	0.001131271	-0.146064533	-0.128439513
12	0	0.001087445	-0.147167647	-0.129533167
12.1	0	0.001044069	-0.148267058	-0.130623121
12.2	0	0.001001138	-0.149362795	-0.131709401
12.3	0	0.000958651	-0.150454886	-0.132792036
12.4	0	0.000916602	-0.151543358	-0.133871053
12.5	0	0.00087499	-0.152628239	-0.13494648
12.6	0	0.00083381	-0.153709554	-0.136018343
12.7	0	0.00079306	-0.154787332	-0.137086669
12.8	0	0.000752736	-0.155861597	-0.138151483
12.9	0	0.000712835	-0.156932375	-0.139212812
13	0	0.000673354	-0.157999693	-0.140270682
13.1	0	0.00063429	-0.159063575	-0.141325116
13.2	0	0.000595639	-0.160124046	-0.142376141
13.3	0	0.000557399	-0.16118113	-0.14342378
13.4	0	0.000519567	-0.162234852	-0.144468059
13.5	0	0.000482139	-0.163285236	-0.145509
13.6	0	0.000445114	-0.164332306	-0.146546628
13.7	0	0.000408487	-0.165376084	-0.147580966
13.8	0	0.000372256	-0.166416594	-0.148612037
13.9	0	0.000336419	-0.167453859	-0.149639863

14	0	0.000300972	-0.168487902	-0.150664469
14.1	0	0.000265913	-0.169518743	-0.151685875
14.2	0	0.00023124	-0.170546407	-0.152704103
14.3	0	0.000196948	-0.171570914	-0.153719177
14.4	0	0.000163037	-0.172592286	-0.154731116
14.5	0	0.000129502	-0.173610544	-0.155739943
14.6	0	0.0000963422	-0.17462571	-0.156745678
14.7	0	0.0000635543	-0.175637803	-0.157748343
14.8	0	0.000031136	-0.176646845	-0.158747957
14.9	0	-0.0000009155	-0.177652856	-0.159744542
15	0	-0.0000326023	-0.178655857	-0.160738116
15.1	0	-0.0000639271	-0.179655866	-0.161728701
15.2	0	-0.0000948921	-0.180652904	-0.162716316
15.3	0	-0.0001255	-0.181646989	-0.16370098
15.4	0	-0.000155753	-0.182638143	-0.164682713
15.5	0	-0.000185653	-0.183626382	-0.165661533
15.6	0	-0.000215203	-0.184611727	-0.166637459
15.7	0	-0.000244405	-0.185594196	-0.167610511
15.8	0	-0.000273261	-0.186573806	-0.168580706
15.9	0	-0.000301774	-0.187550578	-0.169548062
16	0	-0.000329945	-0.188524527	-0.170512598
16.1	0	-0.000357777	-0.189495673	-0.171474332
16.2	0	-0.000385272	-0.190464033	-0.172433281
16.3	0	-0.000412432	-0.191429624	-0.173389463
16.4	0	-0.00043926	-0.192392465	-0.174342895
16.5	0	-0.000465757	-0.193352571	-0.175293593
16.6	0	-0.000491925	-0.194309959	-0.176241576
16.7	0	-0.000517767	-0.195264647	-0.17718686
16.8	0	-0.000543284	-0.196216652	-0.17812946
16.9	0	-0.000568479	-0.197165989	-0.179069395
17	0	-0.000593353	-0.198112674	-0.18000668
17.1	0	-0.000617909	-0.199056725	-0.180941331

17.2	0	-0.000642148	-0.199998156	-0.181873363
17.3	0	-0.000666072	-0.200936984	-0.182802794
17.4	0	-0.000689684	-0.201873224	-0.183729639
17.5	0	-0.000712984	-0.202806892	-0.184653912
17.6	0	-0.000735976	-0.203738003	-0.185575629
17.7	0	-0.00075866	-0.204666571	-0.186494806
17.8	0	-0.00078104	-0.205592613	-0.187411457
17.9	0	-0.000803115	-0.206516143	-0.188325598
18	0	-0.000824889	-0.207437176	-0.189237242
18.1	0	-0.000846363	-0.208355726	-0.190146406
18.2	0	-0.000867538	-0.209271808	-0.191053102
18.3	0	-0.000888417	-0.210185436	-0.191957345
18.4	0	-0.000909002	-0.211096624	-0.19285915
18.5	0	-0.000929293	-0.212005386	-0.193758531
18.6	0	-0.000949293	-0.212911736	-0.194655501
18.7	0	-0.000969003	-0.213815689	-0.195550075
18.8	0	-0.000988425	-0.214717256	-0.196442265
18.9	0	-0.001007561	-0.215616453	-0.197332085
19	0	-0.001026412	-0.216513293	-0.19821955
19.1	0	-0.00104498	-0.217407788	-0.199104672
19.2	0	-0.001063266	-0.218299952	-0.199987463
19.3	0	-0.001081272	-0.219189798	-0.200867938
19.4	0	-0.001099	-0.220077339	-0.20174611
19.5	0	-0.001116451	-0.220962588	-0.20262199
19.6	0	-0.001133627	-0.221845557	-0.203495592
19.7	0	-0.001150529	-0.222726258	-0.204366928
19.8	0	-0.001167158	-0.223604705	-0.205236011
19.9	0	-0.001183517	-0.22448091	-0.206102852
20	0	-0.001199606	-0.225354884	-0.206967465

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 800 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.012519656	0.031471049	0.047831823
0.1	0	0.01235208	0.029412615	0.045782863
0.2	0	0.012186312	0.027374209	0.04375393
0.3	0	0.012022352	0.025355167	0.041744361
0.4	0	0.011860197	0.023354869	0.039753536
0.5	0	0.01169984	0.021372735	0.037780875
0.6	0	0.011541268	0.019408221	0.035825833
0.7	0	0.011384467	0.017460814	0.033887898
0.8	0	0.011229419	0.015530033	0.031966589
0.9	0	0.011076105	0.013615421	0.030061449
1	0	0.010924507	0.011716549	0.028172049
1.1	0	0.010774602	0.009833008	0.02629798
1.2	0	0.010626369	0.007964411	0.024438854
1.3	0	0.010479787	0.006110391	0.022594304
1.4	0	0.010334831	0.004270595	0.020763979
1.5	0	0.010191481	0.002444692	0.018947546
1.6	0	0.010049713	0.000632362	0.017144686
1.7	0	0.009909505	-0.001166699	0.015355095
1.8	0	0.009770834	-0.002952783	0.013578481
1.9	0	0.009633678	-0.004726166	0.011814567
2	0	0.009498015	-0.006487118	0.010063085
2.1	0	0.009363823	-0.008235893	0.008323778
2.2	0	0.009231081	-0.009972738	0.006596402
2.3	0	0.009099768	-0.011697889	0.004880719
2.4	0	0.008969863	-0.013411574	0.003176502
2.5	0	0.008841344	-0.015114011	0.001483532
2.6	0	0.008714194	-0.016805412	-0.000198402

2.7	0	0.008588391	-0.01848598	-0.001869503
2.8	0	0.008463916	-0.020155911	-0.003529968
2.9	0	0.008340751	-0.021815395	-0.005179985
3	0	0.008218876	-0.023464614	-0.006819739
3.1	0	0.008098275	-0.025103746	-0.008449405
3.2	0	0.007978928	-0.026732961	-0.010069155
3.3	0	0.007860819	-0.028352425	-0.011679155
3.4	0	0.00774393	-0.0299623	-0.013279565
3.5	0	0.007628245	-0.031562739	-0.014870541
3.6	0	0.007513746	-0.033153894	-0.016452233
3.7	0	0.00740042	-0.034735912	-0.018024787
3.8	0	0.007288248	-0.036308933	-0.019588346
3.9	0	0.007177217	-0.037873096	-0.021143047
4	0	0.007067311	-0.039428534	-0.022689023
4.1	0	0.006958515	-0.040975378	-0.024226405
4.2	0	0.006850816	-0.042513753	-0.025755532
4.3	0	0.006744197	-0.044043783	-0.02727589
4.4	0	0.006638647	-0.045565588	-0.028788234
4.5	0	0.006534152	-0.047079283	-0.03029247
4.6	0	0.006430697	-0.048584982	-0.03178871
4.7	0	0.006328271	-0.050082796	-0.033277065
4.8	0	0.00622686	-0.051572832	-0.034757643
4.9	0	0.006126452	-0.053055195	-0.036230549
5	0	0.006027035	-0.054529987	-0.037695884
5.1	0	0.005928597	-0.055997309	-0.039153748
5.2	0	0.005831125	-0.057457256	-0.04060424
5.3	0	0.005734609	-0.058909926	-0.042047454
5.4	0	0.005639038	-0.060355409	-0.043483482
5.5	0	0.005544399	-0.061793798	-0.044912416
5.6	0	0.005450683	-0.063225179	-0.046334344
5.7	0	0.005357879	-0.064649641	-0.047749352
5.8	0	0.005265976	-0.066067267	-0.049157525

5.9	0	0.005174964	-0.067478141	-0.050558946
6	0	0.005084832	-0.068882342	-0.051953695
6.1	0	0.004995573	-0.07027995	-0.053341852
6.2	0	0.004907174	-0.071671043	-0.054723494
6.3	0	0.004819628	-0.073055696	-0.056098697
6.4	0	0.004732924	-0.074433983	-0.057467534
6.5	0	0.004647054	-0.075805977	-0.058830079
6.6	0	0.004562009	-0.077171749	-0.060186403
6.7	0	0.00447778	-0.078531369	-0.061536575
6.8	0	0.004394357	-0.079884905	-0.062880664
6.9	0	0.004311734	-0.081232424	-0.064218736
7	0	0.004229901	-0.082573991	-0.065550857
7.1	0	0.00414885	-0.083909671	-0.066877091
7.2	0	0.004068573	-0.085239526	-0.068197502
7.3	0	0.003989062	-0.08656362	-0.069512151
7.4	0	0.00391031	-0.087882011	-0.070821098
7.5	0	0.003832308	-0.08919476	-0.072124405
7.6	0	0.00375505	-0.090501925	-0.073422127
7.7	0	0.003678528	-0.091803564	-0.074714324
7.8	0	0.003602735	-0.093099732	-0.076001052
7.9	0	0.003527663	-0.094390485	-0.077282364
8	0	0.003453305	-0.095675878	-0.078558317
8.1	0	0.003379655	-0.096955963	-0.079828963
8.2	0	0.003306706	-0.098230793	-0.081094355
8.3	0	0.003234451	-0.099500419	-0.082354543
8.4	0	0.003162884	-0.100764893	-0.08360958
8.5	0	0.003091998	-0.102024262	-0.084859513
8.6	0	0.003021786	-0.103278578	-0.086104393
8.7	0	0.002952243	-0.104527886	-0.087344266
8.8	0	0.002883363	-0.105772236	-0.088579181
8.9	0	0.002815138	-0.107011672	-0.089809184
9	0	0.002747564	-0.108246241	-0.09103432

9.1	0	0.002680635	-0.109475988	-0.092254634
9.2	0	0.002614343	-0.110700956	-0.093470172
9.3	0	0.002548685	-0.11192119	-0.094680975
9.4	0	0.002483654	-0.113136732	-0.095887086
9.5	0	0.002419245	-0.114347624	-0.097088549
9.6	0	0.002355452	-0.115553907	-0.098285404
9.7	0	0.002292271	-0.116755623	-0.099477693
9.8	0	0.002229695	-0.117952812	-0.100665454
9.9	0	0.002167719	-0.119145513	-0.101848729
10	0	0.002106339	-0.120333765	-0.103027555
10.1	0	0.002045548	-0.121517606	-0.104201971
10.2	0	0.001985344	-0.122697074	-0.105372016
10.3	0	0.001925719	-0.123872207	-0.106537726
10.4	0	0.001866671	-0.125043042	-0.107699137
10.5	0	0.001808192	-0.126209613	-0.108856287
10.6	0	0.00175028	-0.127371957	-0.11000921
10.7	0	0.00169293	-0.128530109	-0.111157942
10.8	0	0.001636136	-0.129684104	-0.112302518
10.9	0	0.001579894	-0.130833976	-0.113442971
11	0	0.0015242	-0.131979757	-0.114579335
11.1	0	0.00146905	-0.133121482	-0.115711643
11.2	0	0.001414439	-0.134259184	-0.116839928
11.3	0	0.001360363	-0.135392893	-0.117964222
11.4	0	0.001306817	-0.136522643	-0.119084558
11.5	0	0.001253798	-0.137648464	-0.120200965
11.6	0	0.001201301	-0.138770388	-0.121313476
11.7	0	0.001149323	-0.139888444	-0.12242212
11.8	0	0.001097859	-0.141002663	-0.123526929
11.9	0	0.001046905	-0.142113075	-0.12462793
12	0	0.000996458	-0.143219709	-0.125725155
12.1	0	0.000946513	-0.144322594	-0.126818631
12.2	0	0.000897068	-0.145421759	-0.127908388

12.3	0	0.000848117	-0.14651723	-0.128994453
12.4	0	0.000799658	-0.147609038	-0.130076854
12.5	0	0.000751686	-0.148697208	-0.131155619
12.6	0	0.000704199	-0.149781768	-0.132230774
12.7	0	0.000657192	-0.150862744	-0.133302348
12.8	0	0.000610662	-0.151940164	-0.134370365
12.9	0	0.000564606	-0.153014053	-0.135434852
13	0	0.00051902	-0.154084437	-0.136495835
13.1	0	0.000473901	-0.155151341	-0.13755334
13.2	0	0.000429245	-0.156214791	-0.13860739
13.3	0	0.00038505	-0.157274811	-0.139658012
13.4	0	0.000341311	-0.158331426	-0.14070523
13.5	0	0.000298026	-0.15938466	-0.141749068
13.6	0	0.000255191	-0.160434536	-0.142789549
13.7	0	0.000212803	-0.16148108	-0.143826698
13.8	0	0.00017086	-0.162524313	-0.144860538
13.9	0	0.000129358	-0.16356426	-0.145891092
14	0	0.0000882938	-0.164600942	-0.146918383
14.1	0	0.0000476647	-0.165634383	-0.147942433
14.2	0	0.0000074677	-0.166664605	-0.148963265
14.3	0	-0.0000323002	-0.167691629	-0.149980901
14.4	0	-0.0000716419	-0.168715478	-0.150995362
14.5	0	-0.00011056	-0.169736173	-0.15200667
14.6	0	-0.000149058	-0.170753736	-0.153014846
14.7	0	-0.000187138	-0.171768187	-0.154019912
14.8	0	-0.000224803	-0.172779547	-0.155021888
14.9	0	-0.000262056	-0.173787836	-0.156020794
15	0	-0.0002989	-0.174793076	-0.157016652
15.1	0	-0.000335336	-0.175795286	-0.158009481
15.2	0	-0.000371369	-0.176794486	-0.158999301
15.3	0	-0.000407	-0.177790696	-0.159986132
15.4	0	-0.000442232	-0.178783936	-0.160969993

15.5	0	-0.000477068	-0.179774223	-0.161950903
15.6	0	-0.000511509	-0.180761579	-0.162928882
15.7	0	-0.00054556	-0.18174602	-0.163903949
15.8	0	-0.000579222	-0.182727567	-0.164876121
15.9	0	-0.000612497	-0.183706237	-0.165845418
16	0	-0.000645389	-0.18468205	-0.166811858
16.1	0	-0.000677898	-0.185655021	-0.167775458
16.2	0	-0.000710029	-0.186625171	-0.168736238
16.3	0	-0.000741783	-0.187592516	-0.169694213
16.4	0	-0.000773163	-0.188557073	-0.170649403
16.5	0	-0.00080417	-0.189518861	-0.171601823
16.6	0	-0.000834808	-0.190477896	-0.172551492
16.7	0	-0.000865078	-0.191434195	-0.173498426
16.8	0	-0.000894982	-0.192387776	-0.174442642
16.9	0	-0.000924524	-0.193338654	-0.175384157
17	0	-0.000953705	-0.194286846	-0.176322987
17.1	0	-0.000982526	-0.195232368	-0.177259148
17.2	0	-0.001010991	-0.196175237	-0.178192657
17.3	0	-0.001039102	-0.197115469	-0.17912353
17.4	0	-0.00106686	-0.198053079	-0.180051782
17.5	0	-0.001094268	-0.198988082	-0.180977428
17.6	0	-0.001121328	-0.199920495	-0.181900486
17.7	0	-0.001148041	-0.200850333	-0.182820969
17.8	0	-0.00117441	-0.201777611	-0.183738893
17.9	0	-0.001200437	-0.202702344	-0.184654273
18	0	-0.001226124	-0.203624547	-0.185567124
18.1	0	-0.001251473	-0.204544234	-0.186477461
18.2	0	-0.001276485	-0.205461421	-0.187385299
18.3	0	-0.001301163	-0.206376121	-0.188290651
18.4	0	-0.001325509	-0.20728835	-0.189193532
18.5	0	-0.001349524	-0.208198121	-0.190093957
18.6	0	-0.00137321	-0.209105448	-0.190991939

18.7	0	-0.00139657	-0.210010346	-0.191887493
18.8	0	-0.001419604	-0.210912828	-0.192780632
18.9	0	-0.001442316	-0.211812907	-0.19367137
19	0	-0.001464705	-0.212710598	-0.19455972
19.1	0	-0.001486776	-0.213605914	-0.195445696
19.2	0	-0.001508529	-0.214498869	-0.196329312
19.3	0	-0.001529965	-0.215389474	-0.19721058
19.4	0	-0.001551087	-0.216277744	-0.198089514
19.5	0	-0.001571897	-0.217163691	-0.198966125
19.6	0	-0.001592395	-0.218047328	-0.199840429
19.7	0	-0.001612585	-0.218928668	-0.200712436
19.8	0	-0.001632467	-0.219807724	-0.20158216
19.9	0	-0.001652043	-0.220684508	-0.202449613
20	0	-0.001671315	-0.221559032	-0.203314808

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 900 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.013728465	0.036206699	0.052424295
0.1	0	0.013547905	0.034139229	0.050366334
0.2	0	0.013368972	0.032091622	0.048328236
0.3	0	0.013191697	0.03006324	0.046309363
0.4	0	0.013016103	0.028053487	0.044309118
0.5	0	0.012842203	0.026061803	0.042326944
0.6	0	0.012670005	0.024087663	0.040362312
0.7	0	0.012499512	0.02213057	0.038414728
0.8	0	0.012330721	0.020190056	0.036483722
0.9	0	0.012163628	0.018265679	0.034568853
1	0	0.011998226	0.016357018	0.032669701
1.1	0	0.011834502	0.014463677	0.030785867

1.2	0	0.011672447	0.012585275	0.028916974
1.3	0	0.011512045	0.010721455	0.027062661
1.4	0	0.011353284	0.008871871	0.025222585
1.5	0	0.011196146	0.007036198	0.023396419
1.6	0	0.011040615	0.005214121	0.021583849
1.7	0	0.010886676	0.003405343	0.019784578
1.8	0	0.010734309	0.001609576	0.017998317
1.9	0	0.010583498	-0.000173453	0.016224794
2	0	0.010434224	-0.001944009	0.014463744
2.1	0	0.01028647	-0.003702344	0.012714916
2.2	0	0.010140217	-0.0054487	0.010978064
2.3	0	0.009995447	-0.007183312	0.009252958
2.4	0	0.009852143	-0.008906405	0.00753937
2.5	0	0.009710285	-0.010618195	0.005837085
2.6	0	0.009569857	-0.012318891	0.004145893
2.7	0	0.009430841	-0.014008695	0.002465593
2.8	0	0.009293218	-0.015687801	0.000795991
2.9	0	0.009156973	-0.017356398	-0.000863102
3	0	0.009022086	-0.019014667	-0.002511868
3.1	0	0.008888543	-0.020662784	-0.004150482
3.2	0	0.008756325	-0.022300919	-0.005779115
3.3	0	0.008625417	-0.023929237	-0.00739793
3.4	0	0.008495803	-0.025547897	-0.009007089
3.5	0	0.008367465	-0.027157055	-0.010606746
3.6	0	0.00824039	-0.028756861	-0.01219705
3.7	0	0.00811456	-0.030347459	-0.013778148
3.8	0	0.007989962	-0.031928992	-0.015350181
3.9	0	0.00786658	-0.033501597	-0.016913286
4	0	0.007744399	-0.035065407	-0.018467597
4.1	0	0.007623405	-0.036620553	-0.020013243
4.2	0	0.007503584	-0.03816716	-0.021550351
4.3	0	0.007384922	-0.039705351	-0.023079044

4.4	0	0.007267405	-0.041235246	-0.024599441
4.5	0	0.00715102	-0.042756961	-0.026111659
4.6	0	0.007035754	-0.044270609	-0.02761581
4.7	0	0.006921593	-0.045776301	-0.029112006
4.8	0	0.006808525	-0.047274144	-0.030600353
4.9	0	0.006696537	-0.048764244	-0.032080958
5	0	0.006585617	-0.050246704	-0.033553922
5.1	0	0.006475753	-0.051721621	-0.035019345
5.2	0	0.006366933	-0.053189095	-0.036477325
5.3	0	0.006259145	-0.054649221	-0.037927957
5.4	0	0.006152379	-0.056102091	-0.039371334
5.5	0	0.006046622	-0.057547797	-0.040807547
5.6	0	0.005941863	-0.058986426	-0.042236685
5.7	0	0.005838093	-0.060418067	-0.043658834
5.8	0	0.005735299	-0.061842803	-0.045074079
5.9	0	0.005633473	-0.063260718	-0.046482503
6	0	0.005532602	-0.064671892	-0.047884188
6.1	0	0.005432678	-0.066076405	-0.049279212
6.2	0	0.00533369	-0.067474336	-0.050667653
6.3	0	0.005235628	-0.068865759	-0.052049588
6.4	0	0.005138483	-0.070250749	-0.053425091
6.5	0	0.005042246	-0.07162938	-0.054794235
6.6	0	0.004946907	-0.073001723	-0.056157091
6.7	0	0.004852456	-0.074367847	-0.057513729
6.8	0	0.004758886	-0.075727821	-0.058864218
6.9	0	0.004666187	-0.077081713	-0.060208626
7	0	0.00457435	-0.078429589	-0.061547017
7.1	0	0.004483367	-0.079771512	-0.062879457
7.2	0	0.00439323	-0.081107547	-0.064206009
7.3	0	0.00430393	-0.082437755	-0.065526735
7.4	0	0.004215459	-0.083762198	-0.066841697
7.5	0	0.004127809	-0.085080936	-0.068150954

7.6	0	0.004040973	-0.086394027	-0.069454564
7.7	0	0.003954942	-0.087701529	-0.070752587
7.8	0	0.003869709	-0.089003498	-0.072045077
7.9	0	0.003785266	-0.090299991	-0.073332092
8	0	0.003701606	-0.091591062	-0.074613685
8.1	0	0.003618722	-0.092876764	-0.075889911
8.2	0	0.003536606	-0.09415715	-0.077160821
8.3	0	0.003455252	-0.095432273	-0.078426468
8.4	0	0.003374653	-0.096702183	-0.079686903
8.5	0	0.003294801	-0.097966929	-0.080942175
8.6	0	0.00321569	-0.099226562	-0.082192334
8.7	0	0.003137314	-0.100481129	-0.083437429
8.8	0	0.003059665	-0.101730679	-0.084677507
8.9	0	0.002982738	-0.102975257	-0.085912614
9	0	0.002906525	-0.10421491	-0.087142797
9.1	0	0.002831022	-0.105449684	-0.088368101
9.2	0	0.002756221	-0.106679622	-0.08958857
9.3	0	0.002682117	-0.107904769	-0.090804249
9.4	0	0.002608703	-0.109125168	-0.09201518
9.5	0	0.002535974	-0.110340861	-0.093221406
9.6	0	0.002463924	-0.11155189	-0.094422969
9.7	0	0.002392547	-0.112758296	-0.09561991
9.8	0	0.002321838	-0.113960119	-0.096812269
9.9	0	0.002251791	-0.115157401	-0.098000087
10	0	0.0021824	-0.116350179	-0.099183402
10.1	0	0.00211366	-0.117538492	-0.100362254
10.2	0	0.002045566	-0.118722379	-0.10153668
10.3	0	0.001978112	-0.119901878	-0.102706718
10.4	0	0.001911294	-0.121077025	-0.103872405
10.5	0	0.001845106	-0.122247856	-0.105033778
10.6	0	0.001779543	-0.123414408	-0.106190872
10.7	0	0.0017146	-0.124576716	-0.107343723

10.8	0	0.001650273	-0.125734814	-0.108492365
10.9	0	0.001586556	-0.126888739	-0.109636834
11	0	0.001523444	-0.128038523	-0.110777163
11.1	0	0.001460933	-0.129184199	-0.111913386
11.2	0	0.001399019	-0.130325801	-0.113045535
11.3	0	0.001337696	-0.131463361	-0.114173643
11.4	0	0.00127696	-0.132596912	-0.115297743
11.5	0	0.001216807	-0.133726485	-0.116417866
11.6	0	0.001157231	-0.134852111	-0.117534043
11.7	0	0.00109823	-0.135973821	-0.118646304
11.8	0	0.001039798	-0.137091646	-0.119754681
11.9	0	0.000981932	-0.138205615	-0.120859204
12	0	0.000924626	-0.139315758	-0.121959901
12.1	0	0.000867878	-0.140422104	-0.123056803
12.2	0	0.000811682	-0.141524683	-0.124149937
12.3	0	0.000756035	-0.142623522	-0.125239333
12.4	0	0.000700932	-0.143718649	-0.126325018
12.5	0	0.000646371	-0.144810093	-0.127407021
12.6	0	0.000592346	-0.145897881	-0.128485369
12.7	0	0.000538854	-0.146982039	-0.129560088
12.8	0	0.000485892	-0.148062595	-0.130631205
12.9	0	0.000433455	-0.149139575	-0.131698748
13	0	0.000381539	-0.150213004	-0.132762741
13.1	0	0.000330142	-0.151282909	-0.13382321
13.2	0	0.00027926	-0.152349315	-0.134880182
13.3	0	0.000228888	-0.153412247	-0.13593368
13.4	0	0.000179023	-0.15447173	-0.13698373
13.5	0	0.000129662	-0.155527788	-0.138030357
13.6	0	0.0000808018	-0.156580446	-0.139073584
13.7	0	0.0000324381	-0.157629727	-0.140113435
13.8	0	-0.0000154319	-0.158675655	-0.141149934
13.9	0	-0.0000628117	-0.159718253	-0.142183105

14	0	-0.000109705	-0.160757545	-0.14321297
14.1	0	-0.000156114	-0.161793553	-0.144239552
14.2	0	-0.000202043	-0.162826299	-0.145262874
14.3	0	-0.000247495	-0.163855807	-0.146282958
14.4	0	-0.000292472	-0.164882098	-0.147299826
14.5	0	-0.000336979	-0.165905193	-0.1483135
14.6	0	-0.000381019	-0.166925115	-0.149324001
14.7	0	-0.000424593	-0.167941884	-0.15033135
14.8	0	-0.000467706	-0.168955523	-0.15133557
14.9	0	-0.000510359	-0.16996605	-0.15233668
15	0	-0.000552557	-0.170973488	-0.153334701
15.1	0	-0.000594303	-0.171977855	-0.154329653
15.2	0	-0.000635598	-0.172979174	-0.155321557
15.3	0	-0.000676446	-0.173977463	-0.156310432
15.4	0	-0.00071685	-0.174972741	-0.157296299
15.5	0	-0.000756813	-0.17596503	-0.158279176
15.6	0	-0.000796337	-0.176954347	-0.159259083
15.7	0	-0.000835424	-0.177940712	-0.160236039
15.8	0	-0.000874079	-0.178924144	-0.161210063
15.9	0	-0.000912303	-0.179904661	-0.162181173
16	0	-0.0009501	-0.180882282	-0.163149388
16.1	0	-0.000987471	-0.181857025	-0.164114727
16.2	0	-0.001024419	-0.182828908	-0.165077206
16.3	0	-0.001060947	-0.18379795	-0.166036845
16.4	0	-0.001097058	-0.184764167	-0.166993661
16.5	0	-0.001132754	-0.185727577	-0.167947671
16.6	0	-0.001168038	-0.186688198	-0.168898893
16.7	0	-0.001202911	-0.187646047	-0.169847343
16.8	0	-0.001237377	-0.188601141	-0.17079304
16.9	0	-0.001271437	-0.189553496	-0.171735999
17	0	-0.001305095	-0.19050313	-0.172676238
17.1	0	-0.001338353	-0.191450058	-0.173613772

17.2	0	-0.001371213	-0.192394297	-0.174548619
17.3	0	-0.001403677	-0.193335863	-0.175480794
17.4	0	-0.001435748	-0.194274773	-0.176410313
17.5	0	-0.001467427	-0.195211042	-0.177337193
17.6	0	-0.001498718	-0.196144685	-0.178261448
17.7	0	-0.001529622	-0.197075718	-0.179183095
17.8	0	-0.001560142	-0.198004157	-0.180102148
17.9	0	-0.00159028	-0.198930017	-0.181018624
18	0	-0.001620038	-0.199853313	-0.181932536
18.1	0	-0.001649418	-0.20077406	-0.182843901
18.2	0	-0.001678422	-0.201692273	-0.183752732
18.3	0	-0.001707053	-0.202607965	-0.184659045
18.4	0	-0.001735312	-0.203521153	-0.185562854
18.5	0	-0.001763202	-0.20443185	-0.186464173
18.6	0	-0.001790725	-0.20534007	-0.187363017
18.7	0	-0.001817882	-0.206245828	-0.1882594
18.8	0	-0.001844677	-0.207149137	-0.189153336
18.9	0	-0.00187111	-0.208050012	-0.190044838
19	0	-0.001897183	-0.208948466	-0.19093392
19.1	0	-0.0019229	-0.209844512	-0.191820596
19.2	0	-0.001948261	-0.210738165	-0.19270488
19.3	0	-0.001973268	-0.211629438	-0.193586785
19.4	0	-0.001997924	-0.212518343	-0.194466323
19.5	0	-0.002022231	-0.213404894	-0.195343509
19.6	0	-0.002046189	-0.214289104	-0.196218355
19.7	0	-0.002069802	-0.215170986	-0.197090873
19.8	0	-0.002093071	-0.216050552	-0.197961078
19.9	0	-0.002115998	-0.216927816	-0.198828981
20	0	-0.002138584	-0.217802789	-0.199694595

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1000 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.01497464	0.040872936	0.05695879
0.1	0	0.014781224	0.038797337	0.054892642
0.2	0	0.014589233	0.036741397	0.052846153
0.3	0	0.014398726	0.034704507	0.050818714
0.4	0	0.014209753	0.032686096	0.048809753
0.5	0	0.01402235	0.030685627	0.046818734
0.6	0	0.013836545	0.028702593	0.044845149
0.7	0	0.013652359	0.026736515	0.042888521
0.8	0	0.013469806	0.024786941	0.040948397
0.9	0	0.013288897	0.022853442	0.039024347
1	0	0.013109636	0.020935612	0.037115965
1.1	0	0.012932024	0.019033063	0.035222865
1.2	0	0.01275606	0.017145426	0.033344677
1.3	0	0.01258174	0.015272352	0.03148105
1.4	0	0.012409058	0.013413505	0.029631651
1.5	0	0.012238006	0.011568565	0.027796158
1.6	0	0.012068574	0.009737226	0.025974267
1.7	0	0.011900752	0.007919195	0.024165683
1.8	0	0.011734527	0.006114191	0.022370125
1.9	0	0.011569888	0.004321945	0.020587325
2	0	0.011406821	0.002542198	0.018817024
2.1	0	0.011245312	0.000774701	0.017058973
2.2	0	0.011085347	-0.000980785	0.015312932
2.3	0	0.010926912	-0.002724491	0.013578672
2.4	0	0.010769991	-0.004456637	0.01185597
2.5	0	0.010614569	-0.006177439	0.010144612
2.6	0	0.010460631	-0.007887102	0.008444393

2.7	0	0.010308162	-0.009585826	0.006755113
2.8	0	0.010157146	-0.011273803	0.005076579
2.9	0	0.010007568	-0.012951219	0.003408605
3	0	0.009859412	-0.014618256	0.001751011
3.1	0	0.009712664	-0.016275085	0.000103624
3.2	0	0.009567308	-0.017921877	-0.001533727
3.3	0	0.009423328	-0.019558795	-0.003161204
3.4	0	0.00928071	-0.021185998	-0.004778965
3.5	0	0.009139439	-0.022803638	-0.006387165
3.6	0	0.0089995	-0.024411866	-0.007985953
3.7	0	0.008860879	-0.026010826	-0.009575474
3.8	0	0.00872356	-0.027600658	-0.011155868
3.9	0	0.008587531	-0.029181501	-0.012727271
4	0	0.008452776	-0.030753485	-0.014289818
4.1	0	0.008319281	-0.032316742	-0.015843636
4.2	0	0.008187034	-0.033871396	-0.017388853
4.3	0	0.00805602	-0.035417569	-0.01892559
4.4	0	0.007926226	-0.036955382	-0.020453966
4.5	0	0.007797639	-0.03848495	-0.021974098
4.6	0	0.007670246	-0.040006386	-0.023486099
4.7	0	0.007544034	-0.0415198	-0.024990079
4.8	0	0.00741899	-0.043025301	-0.026486145
4.9	0	0.007295103	-0.044522992	-0.027974403
5	0	0.007172359	-0.046012977	-0.029454954
5.1	0	0.007050747	-0.047495354	-0.030927899
5.2	0	0.006930255	-0.048970222	-0.032393335
5.3	0	0.00681087	-0.050437676	-0.033851357
5.4	0	0.006692583	-0.051897809	-0.035302058
5.5	0	0.006575381	-0.053350711	-0.03674553
5.6	0	0.006459253	-0.054796472	-0.03818186
5.7	0	0.006344188	-0.056235178	-0.039611137
5.8	0	0.006230175	-0.057666915	-0.041033444

5.9	0	0.006117204	-0.059091765	-0.042448866
6	0	0.006005265	-0.060509809	-0.043857482
6.1	0	0.005894346	-0.061921128	-0.045259374
6.2	0	0.005784437	-0.063325798	-0.046654618
6.3	0	0.005675553	-0.064723898	-0.048043291
6.4	0	0.005567613	-0.0661155	-0.049425467
6.5	0	0.005460678	-0.067500678	-0.050801221
6.6	0	0.005354714	-0.068879504	-0.052170622
6.7	0	0.005249712	-0.070252048	-0.053533743
6.8	0	0.005145663	-0.071618379	-0.054890651
6.9	0	0.005042558	-0.072978565	-0.056241414
7	0	0.004940388	-0.074332671	-0.057586098
7.1	0	0.004839144	-0.075680762	-0.058924768
7.2	0	0.004738817	-0.077022903	-0.060257488
7.3	0	0.004639399	-0.078359155	-0.06158432
7.4	0	0.004540881	-0.07968958	-0.062905325
7.5	0	0.004443255	-0.081014238	-0.064220565
7.6	0	0.004346513	-0.082333189	-0.065530097
7.7	0	0.004250646	-0.083646489	-0.06683398
7.8	0	0.004155648	-0.084954196	-0.06813227
7.9	0	0.004061509	-0.086256366	-0.069425024
8	0	0.003968222	-0.087553055	-0.070712297
8.1	0	0.00387578	-0.088844315	-0.071994142
8.2	0	0.003784175	-0.090130199	-0.073270613
8.3	0	0.0036934	-0.091410761	-0.074541761
8.4	0	0.003603447	-0.092686051	-0.075807639
8.5	0	0.003514309	-0.09395612	-0.077068295
8.6	0	0.003425979	-0.095221017	-0.078323781
8.7	0	0.003338451	-0.09648079	-0.079574143
8.8	0	0.003251717	-0.097735488	-0.080819431
8.9	0	0.00316577	-0.098985158	-0.082059692
9	0	0.003080605	-0.100229846	-0.083294972

9.1	0	0.002996213	-0.101469598	-0.084525315
9.2	0	0.00291259	-0.102704458	-0.085750768
9.3	0	0.002829727	-0.10393447	-0.086971375
9.4	0	0.00274762	-0.105159679	-0.088187178
9.5	0	0.002666261	-0.106380127	-0.089398221
9.6	0	0.002585646	-0.107595856	-0.090604545
9.7	0	0.002505766	-0.108806907	-0.091806193
9.8	0	0.002426618	-0.110013321	-0.093003205
9.9	0	0.002348194	-0.111215139	-0.094195621
10	0	0.002270489	-0.1124124	-0.095383481
10.1	0	0.002193497	-0.113605143	-0.096566823
10.2	0	0.002117212	-0.114793406	-0.097745687
10.3	0	0.00204163	-0.115977228	-0.09892011
10.4	0	0.001966744	-0.117156646	-0.10009013
10.5	0	0.001892549	-0.118331695	-0.101255783
10.6	0	0.001819039	-0.119502414	-0.102417105
10.7	0	0.00174621	-0.120668837	-0.103574132
10.8	0	0.001674055	-0.121830999	-0.1047269
10.9	0	0.001602571	-0.122988936	-0.105875443
11	0	0.001531751	-0.124142682	-0.107019795
11.1	0	0.001461591	-0.125292269	-0.10815999
11.2	0	0.001392085	-0.126437733	-0.109296062
11.3	0	0.00132323	-0.127579104	-0.110428043
11.4	0	0.001255019	-0.128716417	-0.111555965
11.5	0	0.001187448	-0.129849702	-0.112679861
11.6	0	0.001120513	-0.130978991	-0.113799762
11.7	0	0.001054209	-0.132104316	-0.1149157
11.8	0	0.00098853	-0.133225707	-0.116027704
11.9	0	0.000923474	-0.134343194	-0.117135805
12	0	0.000859034	-0.135456807	-0.118240033
12.1	0	0.000795207	-0.136566576	-0.119340418
12.2	0	0.000731988	-0.137672529	-0.120436988

12.3	0	0.000669373	-0.138774696	-0.121529773
12.4	0	0.000607357	-0.139873105	-0.1226188
12.5	0	0.000545937	-0.140967783	-0.123704098
12.6	0	0.000485108	-0.142058759	-0.124785694
12.7	0	0.000424866	-0.14314606	-0.125863616
12.8	0	0.000365207	-0.144229713	-0.126937891
12.9	0	0.000306127	-0.145309743	-0.128008545
13	0	0.000247621	-0.146386179	-0.129075604
13.1	0	0.000189687	-0.147459045	-0.130139094
13.2	0	0.000132319	-0.148528367	-0.131199042
13.3	0	0.0000755146	-0.149594171	-0.132255472
13.4	0	0.0000192693	-0.150656481	-0.13330841
13.5	0	-0.0000364204	-0.151715322	-0.13435788
13.6	0	-0.0000915582	-0.15277072	-0.135403906
13.7	0	-0.000146148	-0.153822697	-0.136446514
13.8	0	-0.000200193	-0.154871278	-0.137485726
13.9	0	-0.000253698	-0.155916487	-0.138521566
14	0	-0.000306665	-0.156958346	-0.139554058
14.1	0	-0.000359099	-0.157996879	-0.140583225
14.2	0	-0.000411002	-0.159032108	-0.141609089
14.3	0	-0.000462378	-0.160064056	-0.142631673
14.4	0	-0.000513232	-0.161092746	-0.143650999
14.5	0	-0.000563565	-0.162118199	-0.14466709
14.6	0	-0.000613382	-0.163140437	-0.145679966
14.7	0	-0.000662685	-0.164159481	-0.14668965
14.8	0	-0.000711478	-0.165175353	-0.147696162
14.9	0	-0.000759764	-0.166188074	-0.148699524
15	0	-0.000807547	-0.167197664	-0.149699757
15.1	0	-0.000854829	-0.168204145	-0.150696881
15.2	0	-0.000901614	-0.169207536	-0.151690916
15.3	0	-0.000947905	-0.170207858	-0.152681883
15.4	0	-0.000993704	-0.17120513	-0.153669802

15.5	0	-0.001039016	-0.172199372	-0.154654692
15.6	0	-0.001083842	-0.173190605	-0.155636572
15.7	0	-0.001128187	-0.174178846	-0.156615462
15.8	0	-0.001172052	-0.175164115	-0.157591382
15.9	0	-0.001215441	-0.176146431	-0.158564349
16	0	-0.001258356	-0.177125813	-0.159534383
16.1	0	-0.001300801	-0.178102279	-0.160501502
16.2	0	-0.001342778	-0.179075847	-0.161465724
16.3	0	-0.001384291	-0.180046535	-0.162427068
16.4	0	-0.001425341	-0.181014362	-0.163385551
16.5	0	-0.001465933	-0.181979345	-0.164341191
16.6	0	-0.001506067	-0.182941501	-0.165294005
16.7	0	-0.001545747	-0.183900849	-0.166244012
16.8	0	-0.001584977	-0.184857404	-0.167191227
16.9	0	-0.001623757	-0.185811185	-0.168135669
17	0	-0.001662092	-0.186762207	-0.169077354
17.1	0	-0.001699982	-0.187710488	-0.170016298
17.2	0	-0.001737433	-0.188656045	-0.170952519
17.3	0	-0.001774445	-0.189598893	-0.171886032
17.4	0	-0.001811021	-0.190539048	-0.172816854
17.5	0	-0.001847163	-0.191476527	-0.173745001
17.6	0	-0.001882875	-0.192411346	-0.174670488
17.7	0	-0.001918159	-0.19334352	-0.175593331
17.8	0	-0.001953016	-0.194273064	-0.176513546
17.9	0	-0.00198745	-0.195199995	-0.177431149
18	0	-0.002021462	-0.196124328	-0.178346154
18.1	0	-0.002055056	-0.197046077	-0.179258577
18.2	0	-0.002088233	-0.197965257	-0.180168432
18.3	0	-0.002120996	-0.198881884	-0.181075735
18.4	0	-0.002153347	-0.199795972	-0.1819805
18.5	0	-0.002185288	-0.200707536	-0.182882742
18.6	0	-0.002216822	-0.20161659	-0.183782475

18.7	0	-0.002247951	-0.202523148	-0.184679713
18.8	0	-0.002278676	-0.203427225	-0.185574471
18.9	0	-0.002309001	-0.204328834	-0.186466762
19	0	-0.002338927	-0.205227989	-0.187356601
19.1	0	-0.002368457	-0.206124705	-0.188244002
19.2	0	-0.002397592	-0.207018995	-0.189128977
19.3	0	-0.002426335	-0.207910872	-0.190011541
19.4	0	-0.002454688	-0.208800349	-0.190891706
19.5	0	-0.002482653	-0.209687441	-0.191769487
19.6	0	-0.002510232	-0.21057216	-0.192644895
19.7	0	-0.002537426	-0.211454519	-0.193517945
19.8	0	-0.002564239	-0.212334531	-0.194388649
19.9	0	-0.002590671	-0.213212208	-0.195257021
20	0	-0.002616726	-0.214087565	-0.196123072

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1100 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.016252031	0.04549095	0.061425277
0.1	0	0.016046147	0.043408136	0.059351928
0.2	0	0.015841459	0.041344737	0.057297995
0.3	0	0.015638057	0.039300173	0.055262898
0.4	0	0.015436016	0.0372739	0.053246092
0.5	0	0.015235396	0.035265405	0.051247063
0.6	0	0.015036248	0.033274201	0.049265326
0.7	0	0.014838611	0.031299829	0.047300422
0.8	0	0.014642517	0.029341854	0.045351914
0.9	0	0.01444799	0.027399863	0.043419391
1	0	0.014255049	0.025473461	0.041502457
1.1	0	0.014063709	0.023562275	0.039600739

1.2	0	0.013873978	0.021665948	0.03771388
1.3	0	0.013685864	0.019784139	0.035841539
1.4	0	0.013499368	0.017916521	0.03398339
1.5	0	0.013314492	0.016062785	0.032139123
1.6	0	0.013131234	0.014222631	0.030308438
1.7	0	0.012949589	0.012395774	0.028491049
1.8	0	0.012769554	0.010581938	0.026686683
1.9	0	0.01259112	0.008780861	0.024895075
2	0	0.012414279	0.006992289	0.023115972
2.1	0	0.012239023	0.005215978	0.02134913
2.2	0	0.012065342	0.003451693	0.019594315
2.3	0	0.011893225	0.001699209	0.0178513
2.4	0	0.011722661	-0.0000416933	0.016119867
2.5	0	0.011553639	-0.001771224	0.014399806
2.6	0	0.011386145	-0.003489586	0.012690913
2.7	0	0.011220167	-0.005196977	0.010992992
2.8	0	0.011055693	-0.006893585	0.009305853
2.9	0	0.01089271	-0.008579594	0.007629313
3	0	0.010731204	-0.010255183	0.005963194
3.1	0	0.010571161	-0.011920523	0.004307323
3.2	0	0.01041257	-0.013575782	0.002661534
3.3	0	0.010255415	-0.01522112	0.001025665
3.4	0	0.010099683	-0.016856696	-0.000600441
3.5	0	0.009945361	-0.018482661	-0.002216937
3.6	0	0.009792436	-0.020099163	-0.00382397
3.7	0	0.009640894	-0.021706345	-0.005421683
3.8	0	0.00949072	-0.023304348	-0.007010217
3.9	0	0.009341903	-0.024893307	-0.008589707
4	0	0.009194429	-0.026473354	-0.010160286
4.1	0	0.009048284	-0.028044617	-0.011722081
4.2	0	0.008903456	-0.029607222	-0.013275217
4.3	0	0.008759931	-0.03116129	-0.014819816

4.4	0	0.008617696	-0.032706939	-0.016355998
4.5	0	0.00847674	-0.034244286	-0.017883876
4.6	0	0.008337049	-0.035773442	-0.019403565
4.7	0	0.008198611	-0.037294519	-0.020915174
4.8	0	0.008061414	-0.038807622	-0.022418809
4.9	0	0.007925445	-0.040312856	-0.023914577
5	0	0.007790693	-0.041810324	-0.025402577
5.1	0	0.007657145	-0.043300124	-0.026882911
5.2	0	0.00752479	-0.044782355	-0.028355675
5.3	0	0.007393616	-0.046257111	-0.029820965
5.4	0	0.007263612	-0.047724485	-0.031278873
5.5	0	0.007134767	-0.049184568	-0.03272949
5.6	0	0.007007068	-0.050637448	-0.034172905
5.7	0	0.006880507	-0.052083213	-0.035609205
5.8	0	0.00675507	-0.053521948	-0.037038474
5.9	0	0.006630749	-0.054953734	-0.038460796
6	0	0.006507532	-0.056378654	-0.039876252
6.1	0	0.006385409	-0.057796788	-0.041284921
6.2	0	0.006264369	-0.059208212	-0.042686882
6.3	0	0.006144403	-0.060613004	-0.044082211
6.4	0	0.0060255	-0.062011239	-0.045470981
6.5	0	0.005907651	-0.063402988	-0.046853268
6.6	0	0.005790845	-0.064788325	-0.048229143
6.7	0	0.005675075	-0.066167319	-0.049598675
6.8	0	0.005560328	-0.06754004	-0.050961934
6.9	0	0.005446598	-0.068906555	-0.052318988
7	0	0.005333874	-0.070266931	-0.053669903
7.1	0	0.005222147	-0.071621232	-0.055014743
7.2	0	0.005111408	-0.072969522	-0.056353573
7.3	0	0.005001649	-0.074311864	-0.057686456
7.4	0	0.004892861	-0.07564832	-0.059013453
7.5	0	0.004785035	-0.07697895	-0.060334624

7.6	0	0.004678163	-0.078303813	-0.061650028
7.7	0	0.004572236	-0.079622967	-0.062959724
7.8	0	0.004467247	-0.080936469	-0.064263769
7.9	0	0.004363187	-0.082244376	-0.065562219
8	0	0.004260048	-0.083546743	-0.06685513
8.1	0	0.004157822	-0.084843624	-0.068142554
8.2	0	0.004056502	-0.086135072	-0.069424547
8.3	0	0.003956079	-0.08742114	-0.070701159
8.4	0	0.003856547	-0.088701878	-0.071972443
8.5	0	0.003757897	-0.089977339	-0.073238449
8.6	0	0.003660123	-0.09124757	-0.074499227
8.7	0	0.003563217	-0.092512622	-0.075754826
8.8	0	0.003467172	-0.093772543	-0.077005294
8.9	0	0.003371981	-0.095027379	-0.078250678
9	0	0.003277637	-0.096277177	-0.079491025
9.1	0	0.003184132	-0.097521984	-0.080726381
9.2	0	0.003091461	-0.098761844	-0.08195679
9.3	0	0.002999616	-0.099996802	-0.083182298
9.4	0	0.002908591	-0.101226901	-0.084402948
9.5	0	0.00281838	-0.102452185	-0.085618783
9.6	0	0.002728975	-0.103672696	-0.086829846
9.7	0	0.002640371	-0.104888475	-0.088036178
9.8	0	0.002552561	-0.106099563	-0.089237819
9.9	0	0.002465539	-0.107306002	-0.090434812
10	0	0.002379298	-0.108507831	-0.091627195
10.1	0	0.002293834	-0.109705089	-0.092815008
10.2	0	0.002209139	-0.110897815	-0.09399829
10.3	0	0.002125209	-0.112086048	-0.095177078
10.4	0	0.002042036	-0.113269823	-0.096351411
10.5	0	0.001959616	-0.11444918	-0.097521325
10.6	0	0.001877942	-0.115624154	-0.098686857
10.7	0	0.00179701	-0.11679478	-0.099848042

10.8	0	0.001716813	-0.117961096	-0.101004917
10.9	0	0.001637346	-0.119123135	-0.102157517
11	0	0.001558603	-0.120280932	-0.103305875
11.1	0	0.00148058	-0.121434521	-0.104450025
11.2	0	0.001403271	-0.122583936	-0.105590003
11.3	0	0.001326671	-0.12372921	-0.106725839
11.4	0	0.001250774	-0.124870375	-0.107857568
11.5	0	0.001175576	-0.126007463	-0.108985221
11.6	0	0.001101072	-0.127140507	-0.11010883
11.7	0	0.001027256	-0.128269538	-0.111228426
11.8	0	0.000954124	-0.129394586	-0.112344041
11.9	0	0.00088167	-0.130515683	-0.113455705
12	0	0.000809891	-0.131632857	-0.114563448
12.1	0	0.00073878	-0.13274614	-0.115667299
12.2	0	0.000668335	-0.13385556	-0.116767289
12.3	0	0.000598549	-0.134961146	-0.117863445
12.4	0	0.000529419	-0.136062928	-0.118955798
12.5	0	0.000460939	-0.137160932	-0.120044374
12.6	0	0.000393106	-0.138255188	-0.121129202
12.7	0	0.000325915	-0.139345722	-0.12221031
12.8	0	0.000259362	-0.140432561	-0.123287724
12.9	0	0.000193442	-0.141515734	-0.124361472
13	0	0.00012815	-0.142595266	-0.12543158
13.1	0	0.0000634839	-0.143671183	-0.126498073
13.2	0	-0.0000005619	-0.144743511	-0.127560979
13.3	0	-0.0000639914	-0.145812276	-0.128620323
13.4	0	-0.000126808	-0.146877504	-0.12967613
13.5	0	-0.000189017	-0.147939218	-0.130728424
13.6	0	-0.000250621	-0.148997444	-0.131777231
13.7	0	-0.000311625	-0.150052207	-0.132822575
13.8	0	-0.000372033	-0.151103529	-0.13386448
13.9	0	-0.000431848	-0.152151436	-0.13490297

14	0	-0.000491074	-0.15319595	-0.135938069
14.1	0	-0.000549715	-0.154237095	-0.136969799
14.2	0	-0.000607775	-0.155274894	-0.137998184
14.3	0	-0.000665258	-0.156309369	-0.139023247
14.4	0	-0.000722166	-0.157340543	-0.140045009
14.5	0	-0.000778504	-0.158368439	-0.141063493
14.6	0	-0.000834276	-0.159393078	-0.142078722
14.7	0	-0.000889485	-0.160414482	-0.143090716
14.8	0	-0.000944134	-0.161432672	-0.144099498
14.9	0	-0.000998227	-0.16244767	-0.145105088
15	0	-0.001051767	-0.163459496	-0.146107509
15.1	0	-0.001104758	-0.164468172	-0.147106779
15.2	0	-0.001157203	-0.165473718	-0.14810292
15.3	0	-0.001209106	-0.166476154	-0.149095953
15.4	0	-0.001260469	-0.167475501	-0.150085897
15.5	0	-0.001311297	-0.168471778	-0.151072772
15.6	0	-0.001361591	-0.169465005	-0.152056598
15.7	0	-0.001411357	-0.170455202	-0.153037395
15.8	0	-0.001460595	-0.171442387	-0.154015182
15.9	0	-0.001509311	-0.172426581	-0.154989977
16	0	-0.001557507	-0.173407801	-0.1559618
16.1	0	-0.001605186	-0.174386066	-0.156930669
16.2	0	-0.00165235	-0.175361395	-0.157896603
16.3	0	-0.001699004	-0.176333806	-0.15885962
16.4	0	-0.00174515	-0.177303318	-0.159819739
16.5	0	-0.001790791	-0.178269947	-0.160776976
16.6	0	-0.00183593	-0.179233712	-0.161731351
16.7	0	-0.00188057	-0.180194631	-0.16268288
16.8	0	-0.001924713	-0.181152721	-0.16363158
16.9	0	-0.001968364	-0.182107998	-0.16457747
17	0	-0.002011523	-0.183060481	-0.165520566
17.1	0	-0.002054195	-0.184010185	-0.166460884

17.2	0	-0.002096382	-0.184957128	-0.167398442
17.3	0	-0.002138086	-0.185901326	-0.168333256
17.4	0	-0.002179311	-0.186842795	-0.169265343
17.5	0	-0.002220059	-0.187781552	-0.170194718
17.6	0	-0.002260334	-0.188717612	-0.171121398
17.7	0	-0.002300136	-0.189650992	-0.172045399
17.8	0	-0.00233947	-0.190581708	-0.172966736
17.9	0	-0.002378337	-0.191509774	-0.173885425
18	0	-0.00241674	-0.192435206	-0.174801481
18.1	0	-0.002454682	-0.19335802	-0.17571492
18.2	0	-0.002492166	-0.194278231	-0.176625757
18.3	0	-0.002529193	-0.195195853	-0.177534006
18.4	0	-0.002565767	-0.196110902	-0.178439684
18.5	0	-0.00260189	-0.197023393	-0.179342803
18.6	0	-0.002637563	-0.197933339	-0.18024338
18.7	0	-0.002672791	-0.198840755	-0.181141428
18.8	0	-0.002707574	-0.199745656	-0.182036962
18.9	0	-0.002741915	-0.200648056	-0.182929995
19	0	-0.002775818	-0.201547969	-0.183820543
19.1	0	-0.002809283	-0.202445408	-0.184708619
19.2	0	-0.002842314	-0.203340389	-0.185594236
19.3	0	-0.002874912	-0.204232923	-0.186477409
19.4	0	-0.002907081	-0.205123025	-0.187358151
19.5	0	-0.002938821	-0.206010709	-0.188236475
19.6	0	-0.002970136	-0.206895987	-0.189112395
19.7	0	-0.003001027	-0.207778872	-0.189985923
19.8	0	-0.003031498	-0.208659379	-0.190857074
19.9	0	-0.003061549	-0.209537519	-0.19172586
20	0	-0.003091183	-0.210413306	-0.192592293

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1200 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.017555738	0.050039456	0.065835837
0.1	0	0.01733791	0.047950228	0.063756032
0.2	0	0.017121028	0.045880145	0.061695371
0.3	0	0.016905213	0.043828657	0.059653306
0.4	0	0.016690566	0.041795247	0.057629318
0.5	0	0.016477173	0.039779425	0.055622919
0.6	0	0.016265105	0.037780728	0.053633644
0.7	0	0.016054419	0.035798714	0.051661054
0.8	0	0.015845166	0.033832968	0.04970473
0.9	0	0.015637386	0.03188309	0.047764276
1	0	0.015431111	0.029948704	0.045839313
1.1	0	0.015226369	0.028029446	0.043929479
1.2	0	0.015023182	0.026124972	0.042034429
1.3	0	0.014821565	0.024234953	0.040153833
1.4	0	0.014621532	0.022359073	0.038287377
1.5	0	0.014423092	0.020497029	0.036434757
1.6	0	0.014226252	0.018648532	0.034595684
1.7	0	0.014031015	0.016813303	0.032769879
1.8	0	0.013837382	0.014991074	0.030957074
1.9	0	0.013645353	0.01318159	0.029157013
2	0	0.013454926	0.0113846	0.027369448
2.1	0	0.013266097	0.009599869	0.025594141
2.2	0	0.01307886	0.007827166	0.023830862
2.3	0	0.01289321	0.006066269	0.022079389
2.4	0	0.01270914	0.004316964	0.020339508
2.5	0	0.012526641	0.002579046	0.018611014
2.6	0	0.012345705	0.000852313	0.016893706

2.7	0	0.012166322	-0.000863426	0.015187391
2.8	0	0.011988483	-0.002568358	0.013491883
2.9	0	0.011812177	-0.004262664	0.011807
3	0	0.011637393	-0.00594652	0.010132568
3.1	0	0.01146412	-0.007620095	0.008468417
3.2	0	0.011292348	-0.009283554	0.006814382
3.3	0	0.011122063	-0.010937056	0.005170303
3.4	0	0.010953256	-0.012580756	0.003536026
3.5	0	0.010785913	-0.014214806	0.0019114
3.6	0	0.010620022	-0.015839351	0.000296279
3.7	0	0.010455573	-0.017454532	-0.001309479
3.8	0	0.010292551	-0.01906049	-0.002906014
3.9	0	0.010130946	-0.020657357	-0.004493458
4	0	0.009970745	-0.022245265	-0.006071943
4.1	0	0.009811936	-0.023824341	-0.007641596
4.2	0	0.009654506	-0.025394708	-0.009202541
4.3	0	0.009498444	-0.026956489	-0.0107549
4.4	0	0.009343737	-0.0285098	-0.012298789
4.5	0	0.009190373	-0.030054757	-0.013834323
4.6	0	0.009038341	-0.03159147	-0.015361615
4.7	0	0.008887628	-0.03312005	-0.016880773
4.8	0	0.008738223	-0.034640603	-0.018391905
4.9	0	0.008590113	-0.036153233	-0.019895114
5	0	0.008443288	-0.037658041	-0.021390501
5.1	0	0.008297736	-0.039155127	-0.022878166
5.2	0	0.008153444	-0.040644587	-0.024358206
5.3	0	0.008010403	-0.042126516	-0.025830715
5.4	0	0.007868601	-0.043601008	-0.027295786
5.5	0	0.007728026	-0.045068151	-0.02875351
5.6	0	0.007588668	-0.046528035	-0.030203975
5.7	0	0.007450515	-0.047980747	-0.031647267
5.8	0	0.007313558	-0.04942637	-0.033083472

5.9	0	0.007177785	-0.050864989	-0.034512671
6	0	0.007043186	-0.052296683	-0.035934948
6.1	0	0.006909751	-0.053721533	-0.03735038
6.2	0	0.006777469	-0.055139617	-0.038759045
6.3	0	0.00664633	-0.05655101	-0.040161021
6.4	0	0.006516323	-0.057955787	-0.041556382
6.5	0	0.006387441	-0.059354022	-0.0429452
6.6	0	0.006259671	-0.060745787	-0.044327548
6.7	0	0.006133006	-0.062131151	-0.045703496
6.8	0	0.006007434	-0.063510184	-0.047073114
6.9	0	0.005882947	-0.064882953	-0.048436468
7	0	0.005759536	-0.066249525	-0.049793625
7.1	0	0.005637191	-0.067609965	-0.05114465
7.2	0	0.005515903	-0.068964337	-0.052489608
7.3	0	0.005395663	-0.070312704	-0.053828561
7.4	0	0.005276462	-0.071655126	-0.05516157
7.5	0	0.005158293	-0.072991666	-0.056488696
7.6	0	0.005041145	-0.074322381	-0.057809999
7.7	0	0.00492501	-0.075647331	-0.059125537
7.8	0	0.00480988	-0.076966572	-0.060435366
7.9	0	0.004695747	-0.078280162	-0.061739544
8	0	0.004582603	-0.079588154	-0.063038126
8.1	0	0.004470439	-0.080890605	-0.064331166
8.2	0	0.004359247	-0.082187566	-0.065618717
8.3	0	0.004249019	-0.083479091	-0.066900833
8.4	0	0.004139749	-0.084765231	-0.068177564
8.5	0	0.004031427	-0.086046037	-0.069448961
8.6	0	0.003924046	-0.087321559	-0.070715076
8.7	0	0.003817599	-0.088591847	-0.071975955
8.8	0	0.003712078	-0.089856947	-0.073231649
8.9	0	0.003607477	-0.091116909	-0.074482204
9	0	0.003503787	-0.092371779	-0.075727667

9.1	0	0.003401002	-0.093621602	-0.076968085
9.2	0	0.003299114	-0.094866425	-0.078203502
9.3	0	0.003198117	-0.096106291	-0.079433964
9.4	0	0.003098004	-0.097341245	-0.080659514
9.5	0	0.002998768	-0.09857133	-0.081880195
9.6	0	0.002900401	-0.099796588	-0.08309605
9.7	0	0.002802899	-0.101017062	-0.084307122
9.8	0	0.002706253	-0.102232793	-0.085513451
9.9	0	0.002610458	-0.103443821	-0.086715078
10	0	0.002515506	-0.104650187	-0.087912043
10.1	0	0.002421393	-0.10585193	-0.089104385
10.2	0	0.002328111	-0.107049089	-0.090292145
10.3	0	0.002235654	-0.108241702	-0.091475359
10.4	0	0.002144017	-0.109429808	-0.092654066
10.5	0	0.002053193	-0.110613443	-0.093828303
10.6	0	0.001963176	-0.111792644	-0.094998107
10.7	0	0.001873961	-0.112967447	-0.096163513
10.8	0	0.001785541	-0.114137889	-0.097324559
10.9	0	0.00169791	-0.115304004	-0.098481278
11	0	0.001611064	-0.116465827	-0.099633706
11.1	0	0.001524997	-0.117623392	-0.100781877
11.2	0	0.001439702	-0.118776733	-0.101925825
11.3	0	0.001355175	-0.119925884	-0.103065582
11.4	0	0.00127141	-0.121070877	-0.104201183
11.5	0	0.001188402	-0.122211745	-0.105332659
11.6	0	0.001106145	-0.123348519	-0.106460042
11.7	0	0.001024634	-0.124481231	-0.107583364
11.8	0	0.000943864	-0.125609913	-0.108702657
11.9	0	0.000863831	-0.126734596	-0.10981795
12	0	0.000784528	-0.127855308	-0.110929274
12.1	0	0.00070595	-0.128972082	-0.112036659
12.2	0	0.000628094	-0.130084945	-0.113140136

12.3	0	0.000550953	-0.131193927	-0.114239732
12.4	0	0.000474524	-0.132299058	-0.115335477
12.5	0	0.000398801	-0.133400365	-0.116427399
12.6	0	0.000323779	-0.134497877	-0.117515527
12.7	0	0.000249455	-0.135591622	-0.118599888
12.8	0	0.000175823	-0.136681626	-0.11968051
12.9	0	0.000102878	-0.137767918	-0.120757419
13	0	0.0000306168	-0.138850523	-0.121830643
13.1	0	-0.0000409658	-0.139929468	-0.122900207
13.2	0	-0.000111874	-0.141004779	-0.123966139
13.3	0	-0.000182113	-0.142076483	-0.125028463
13.4	0	-0.000251686	-0.143144604	-0.126087206
13.5	0	-0.000320598	-0.144209168	-0.127142392
13.6	0	-0.000388852	-0.1452702	-0.128194047
13.7	0	-0.000456454	-0.146327723	-0.129242194
13.8	0	-0.000523407	-0.147381763	-0.130286859
13.9	0	-0.000589716	-0.148432344	-0.131328065
14	0	-0.000655385	-0.149479489	-0.132365837
14.1	0	-0.000720417	-0.150523222	-0.133400197
14.2	0	-0.000784816	-0.151563566	-0.134431168
14.3	0	-0.000848587	-0.152600544	-0.135458775
14.4	0	-0.000911734	-0.153634179	-0.136483039
14.5	0	-0.000974259	-0.154664492	-0.137503982
14.6	0	-0.001036168	-0.155691507	-0.138521628
14.7	0	-0.001097464	-0.156715245	-0.139535997
14.8	0	-0.00115815	-0.157735727	-0.140547113
14.9	0	-0.001218231	-0.158752976	-0.141554995
15	0	-0.00127771	-0.159767013	-0.142559666
15.1	0	-0.00133659	-0.160777858	-0.143561146
15.2	0	-0.001394876	-0.161785532	-0.144559456
15.3	0	-0.00145257	-0.162790056	-0.145554617
15.4	0	-0.001509678	-0.16379145	-0.146546648

15.5	0	-0.0015662	-0.164789734	-0.147535571
15.6	0	-0.001622143	-0.165784928	-0.148521404
15.7	0	-0.001677508	-0.166777052	-0.149504168
15.8	0	-0.001732299	-0.167766126	-0.150483883
15.9	0	-0.001786519	-0.168752167	-0.151460566
16	0	-0.001840173	-0.169735196	-0.152434238
16.1	0	-0.001893262	-0.170715231	-0.153404917
16.2	0	-0.001945791	-0.171692292	-0.154372621
16.3	0	-0.001997763	-0.172666396	-0.155337371
16.4	0	-0.00204918	-0.173637561	-0.156299182
16.5	0	-0.002100047	-0.174605807	-0.157258075
16.6	0	-0.002150366	-0.17557115	-0.158214066
16.7	0	-0.00220014	-0.176533608	-0.159167174
16.8	0	-0.002249372	-0.1774932	-0.160117415
16.9	0	-0.002298066	-0.178449942	-0.161064808
17	0	-0.002346224	-0.179403852	-0.16200937
17.1	0	-0.00239385	-0.180354946	-0.162951117
17.2	0	-0.002440946	-0.181303242	-0.163890066
17.3	0	-0.002487515	-0.182248756	-0.164826235
17.4	0	-0.002533561	-0.183191505	-0.165759639
17.5	0	-0.002579086	-0.184131505	-0.166690295
17.6	0	-0.002624093	-0.185068773	-0.16761822
17.7	0	-0.002668585	-0.186003324	-0.168543429
17.8	0	-0.002712564	-0.186935174	-0.169465938
17.9	0	-0.002756034	-0.187864339	-0.170385763
18	0	-0.002798997	-0.188790834	-0.17130292
18.1	0	-0.002841456	-0.189714676	-0.172217424
18.2	0	-0.002883414	-0.19063588	-0.17312929
18.3	0	-0.002924873	-0.19155446	-0.174038534
18.4	0	-0.002965837	-0.192470431	-0.174945171
18.5	0	-0.003006307	-0.193383809	-0.175849215
18.6	0	-0.003046286	-0.194294609	-0.176750681

18.7	0	-0.003085777	-0.195202844	-0.177649584
18.8	0	-0.003124783	-0.196108529	-0.178545938
18.9	0	-0.003163306	-0.197011679	-0.179439758
19	0	-0.003201348	-0.197912308	-0.180331058
19.1	0	-0.003238912	-0.19881043	-0.181219852
19.2	0	-0.003276001	-0.199706059	-0.182106153
19.3	0	-0.003312617	-0.200599209	-0.182989977
19.4	0	-0.003348762	-0.201489893	-0.183871336
19.5	0	-0.003384439	-0.202378125	-0.184750243
19.6	0	-0.003419651	-0.203263918	-0.185626714
19.7	0	-0.003454399	-0.204147286	-0.18650076
19.8	0	-0.003488686	-0.205028243	-0.187372395
19.9	0	-0.003522515	-0.2059068	-0.188241633
20	0	-0.003555887	-0.206782972	-0.189108485

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1300 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.018881183	0.054541242	0.070187607
0.1	0	0.018651729	0.052446412	0.068102182
0.2	0	0.018422945	0.050370422	0.066035595
0.3	0	0.018194983	0.048312753	0.063987331
0.4	0	0.017967971	0.046272915	0.061956898
0.5	0	0.01774202	0.044250444	0.059943832
0.6	0	0.017517221	0.042244899	0.057947692
0.7	0	0.017293655	0.04025586	0.055968059
0.8	0	0.017071388	0.038282929	0.054004534
0.9	0	0.016850478	0.036325726	0.052056737
1	0	0.016630973	0.034383886	0.050124304
1.1	0	0.016412912	0.032457063	0.048206887

1.2	0	0.016196331	0.030544925	0.046304156
1.3	0	0.015981258	0.028647154	0.044415793
1.4	0	0.015767715	0.026763445	0.042541492
1.5	0	0.015555722	0.024893506	0.040680961
1.6	0	0.015345295	0.023037056	0.038833919
1.7	0	0.015136444	0.021193826	0.037000097
1.8	0	0.014929179	0.019363556	0.035179235
1.9	0	0.014723506	0.017545995	0.033371082
2	0	0.014519429	0.015740903	0.031575399
2.1	0	0.014316951	0.013948047	0.029791953
2.2	0	0.014116071	0.012167205	0.028020519
2.3	0	0.013916788	0.010398158	0.026260882
2.4	0	0.013719101	0.0086407	0.024512833
2.5	0	0.013523004	0.006894627	0.022776169
2.6	0	0.013328494	0.005159743	0.021050695
2.7	0	0.013135565	0.003435861	0.019336223
2.8	0	0.01294421	0.001722797	0.017632568
2.9	0	0.012754422	0.0000203725	0.015939554
3	0	0.012566192	-0.001671583	0.014257008
3.1	0	0.012379514	-0.003353237	0.012584763
3.2	0	0.012194378	-0.005024752	0.010922659
3.3	0	0.012010774	-0.006686285	0.009270537
3.4	0	0.011828693	-0.008337987	0.007628244
3.5	0	0.011648125	-0.009980008	0.005995633
3.6	0	0.01146906	-0.011612492	0.00437256
3.7	0	0.011291488	-0.013235579	0.002758883
3.8	0	0.011115397	-0.014849405	0.001154467
3.9	0	0.010940777	-0.016454104	-0.000440822
4	0	0.010767618	-0.018049804	-0.002027112
4.1	0	0.010595908	-0.019636631	-0.003604529
4.2	0	0.010425637	-0.021214709	-0.005173196
4.3	0	0.010256792	-0.022784156	-0.006733234

4.4	0	0.010089364	-0.02434509	-0.008284758
4.5	0	0.009923341	-0.025897624	-0.009827881
4.6	0	0.009758711	-0.027441868	-0.011362716
4.7	0	0.009595464	-0.028977932	-0.01288937
4.8	0	0.009433588	-0.030505921	-0.01440795
4.9	0	0.009273073	-0.032025938	-0.015918557
5	0	0.009113907	-0.033538085	-0.017421294
5.1	0	0.00895608	-0.035042458	-0.018916258
5.2	0	0.00879958	-0.036539156	-0.020403546
5.3	0	0.008644396	-0.038028271	-0.021883253
5.4	0	0.008490518	-0.039509897	-0.023355469
5.5	0	0.008337935	-0.040984123	-0.024820286
5.6	0	0.008186636	-0.042451036	-0.026277791
5.7	0	0.00803661	-0.043910724	-0.027728071
5.8	0	0.007887848	-0.045363271	-0.029171209
5.9	0	0.007740339	-0.046808759	-0.030607289
6	0	0.007594072	-0.048247269	-0.032036391
6.1	0	0.007449037	-0.049678881	-0.033458595
6.2	0	0.007305223	-0.051103671	-0.034873978
6.3	0	0.007162622	-0.052521717	-0.036282616
6.4	0	0.007021223	-0.053933092	-0.037684584
6.5	0	0.006881016	-0.05533787	-0.039079955
6.6	0	0.006741991	-0.056736122	-0.0404688
6.7	0	0.006604139	-0.058127918	-0.04185119
6.8	0	0.00646745	-0.059513328	-0.043227194
6.9	0	0.006331915	-0.06089242	-0.04459688
7	0	0.006197524	-0.062265258	-0.045960312
7.1	0	0.006064269	-0.063631909	-0.047317558
7.2	0	0.005932139	-0.064992437	-0.048668681
7.3	0	0.005801126	-0.066346904	-0.050013742
7.4	0	0.005671221	-0.067695371	-0.051352806
7.5	0	0.005542415	-0.0690379	-0.05268593

7.6	0	0.0054147	-0.070374549	-0.054013175
7.7	0	0.005288066	-0.071705378	-0.0553346
7.8	0	0.005162505	-0.073030443	-0.056650262
7.9	0	0.005038009	-0.0743498	-0.057960216
8	0	0.004914569	-0.075663506	-0.05926452
8.1	0	0.004792177	-0.076971614	-0.060563226
8.2	0	0.004670825	-0.078274179	-0.061856388
8.3	0	0.004550505	-0.079571252	-0.06314406
8.4	0	0.004431209	-0.080862885	-0.064426292
8.5	0	0.004312928	-0.08214913	-0.065703137
8.6	0	0.004195656	-0.083430037	-0.066974643
8.7	0	0.004079384	-0.084705654	-0.06824086
8.8	0	0.003964104	-0.085976031	-0.069501837
8.9	0	0.00384981	-0.087241214	-0.070757621
9	0	0.003736494	-0.088501252	-0.07200826
9.1	0	0.003624148	-0.089756189	-0.073253799
9.2	0	0.003512765	-0.091006072	-0.074494284
9.3	0	0.003402338	-0.092250945	-0.075729759
9.4	0	0.003292859	-0.093490853	-0.07696027
9.5	0	0.003184323	-0.094725838	-0.078185859
9.6	0	0.003076721	-0.095955944	-0.079406569
9.7	0	0.002970047	-0.097181213	-0.080622442
9.8	0	0.002864294	-0.098401685	-0.081833519
9.9	0	0.002759455	-0.099617403	-0.083039842
10	0	0.002655524	-0.100828407	-0.084241451
10.1	0	0.002552495	-0.102034735	-0.085438386
10.2	0	0.00245036	-0.103236427	-0.086630685
10.3	0	0.002349113	-0.104433522	-0.087818387
10.4	0	0.002248748	-0.105626058	-0.089001531
10.5	0	0.002149259	-0.106814072	-0.090180153
10.6	0	0.00205064	-0.107997601	-0.091354291
10.7	0	0.001952883	-0.109176682	-0.09252398

10.8	0	0.001855984	-0.110351349	-0.093689258
10.9	0	0.001759936	-0.11152164	-0.094850159
11	0	0.001664733	-0.112687589	-0.096006718
11.1	0	0.00157037	-0.113849229	-0.09715897
11.2	0	0.00147684	-0.115006596	-0.098306949
11.3	0	0.001384138	-0.116159722	-0.099450688
11.4	0	0.001292259	-0.117308642	-0.100590221
11.5	0	0.001201196	-0.118453386	-0.101725579
11.6	0	0.001110944	-0.119593988	-0.102856795
11.7	0	0.001021497	-0.12073048	-0.103983902
11.8	0	0.000932851	-0.121862892	-0.10510693
11.9	0	0.000845	-0.122991256	-0.10622591
12	0	0.000757937	-0.124115603	-0.107340873
12.1	0	0.00067166	-0.125235962	-0.108451849
12.2	0	0.00058616	-0.126352363	-0.109558868
12.3	0	0.000501435	-0.127464836	-0.110661959
12.4	0	0.000417479	-0.128573409	-0.111761152
12.5	0	0.000334286	-0.129678112	-0.112856474
12.6	0	0.000251852	-0.130778972	-0.113947955
12.7	0	0.000170172	-0.131876018	-0.115035623
12.8	0	0.0000892407	-0.132969278	-0.116119504
12.9	0	0.0000090534	-0.134058778	-0.117199626
13	0	-0.0000703946	-0.135144545	-0.118276017
13.1	0	-0.000149108	-0.136226607	-0.119348702
13.2	0	-0.000227091	-0.137304989	-0.120417709
13.3	0	-0.00030435	-0.138379718	-0.121483063
13.4	0	-0.000380887	-0.139450819	-0.122544789
13.5	0	-0.000456709	-0.140518317	-0.123602914
13.6	0	-0.000531818	-0.141582238	-0.124657463
13.7	0	-0.000606221	-0.142642607	-0.125708459
13.8	0	-0.000679921	-0.143699447	-0.126755928
13.9	0	-0.000752922	-0.144752784	-0.127799894

14	0	-0.000825229	-0.145802641	-0.128840381
14.1	0	-0.000896846	-0.146849042	-0.129877413
14.2	0	-0.000967778	-0.14789201	-0.130911012
14.3	0	-0.001038028	-0.148931568	-0.131941203
14.4	0	-0.001107601	-0.149967739	-0.132968007
14.5	0	-0.001176501	-0.151000547	-0.133991448
14.6	0	-0.001244731	-0.152030012	-0.135011548
14.7	0	-0.001312296	-0.153056159	-0.13602833
14.8	0	-0.0013792	-0.154079007	-0.137041814
14.9	0	-0.001445447	-0.155098579	-0.138052023
15	0	-0.001511041	-0.156114896	-0.139058978
15.1	0	-0.001575985	-0.15712798	-0.1400627
15.2	0	-0.001640284	-0.158137851	-0.14106321
15.3	0	-0.00170394	-0.159144531	-0.14206053
15.4	0	-0.001766959	-0.160148039	-0.143054678
15.5	0	-0.001829343	-0.161148396	-0.144045677
15.6	0	-0.001891096	-0.162145622	-0.145033545
15.7	0	-0.001952223	-0.163139737	-0.146018303
15.8	0	-0.002012726	-0.16413076	-0.14699997
15.9	0	-0.002072609	-0.165118711	-0.147978566
16	0	-0.002131875	-0.166103609	-0.14895411
16.1	0	-0.002190529	-0.167085474	-0.149926621
16.2	0	-0.002248574	-0.168064323	-0.150896117
16.3	0	-0.002306013	-0.169040176	-0.151862619
16.4	0	-0.002362849	-0.170013052	-0.152826143
16.5	0	-0.002419087	-0.170982967	-0.153786708
16.6	0	-0.002474728	-0.171949942	-0.154744333
16.7	0	-0.002529778	-0.172913992	-0.155699035
16.8	0	-0.002584238	-0.173875137	-0.156650832
16.9	0	-0.002638112	-0.174833394	-0.157599742
17	0	-0.002691404	-0.175788779	-0.158545782
17.1	0	-0.002744116	-0.176741311	-0.159488969

17.2	0	-0.002796252	-0.177691006	-0.16042932
17.3	0	-0.002847815	-0.178637882	-0.161366852
17.4	0	-0.002898807	-0.179581954	-0.162301582
17.5	0	-0.002949234	-0.180523239	-0.163233526
17.6	0	-0.002999096	-0.181461755	-0.164162701
17.7	0	-0.003048397	-0.182397516	-0.165089122
17.8	0	-0.003097141	-0.18333054	-0.166012807
17.9	0	-0.00314533	-0.184260842	-0.166933771
18	0	-0.003192967	-0.185188437	-0.16785203
18.1	0	-0.003240055	-0.186113342	-0.168767599
18.2	0	-0.003286597	-0.187035572	-0.169680493
18.3	0	-0.003332596	-0.187955142	-0.170590729
18.4	0	-0.003378055	-0.188872067	-0.171498321
18.5	0	-0.003422976	-0.189786363	-0.172403285
18.6	0	-0.003467363	-0.190698044	-0.173305635
18.7	0	-0.003511217	-0.191607126	-0.174205386
18.8	0	-0.003554543	-0.192513622	-0.175102552
18.9	0	-0.003597342	-0.193417547	-0.175997149
19	0	-0.003639618	-0.194318916	-0.176889191
19.1	0	-0.003681373	-0.195217743	-0.177778691
19.2	0	-0.003722609	-0.196114041	-0.178665664
19.3	0	-0.00376333	-0.197007826	-0.179550124
19.4	0	-0.003803537	-0.19789911	-0.180432085
19.5	0	-0.003843235	-0.198787908	-0.181311156
19.6	0	-0.003882424	-0.199674233	-0.182188563
19.7	0	-0.003921108	-0.200558099	-0.183063108
19.8	0	-0.003959289	-0.201439519	-0.183935208
19.9	0	-0.00399697	-0.202318505	-0.184804876
20	0	-0.004034154	-0.203195073	-0.185672126

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1400 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.020225719	0.05897898	0.074484048
0.1	0	0.019985318	0.056879377	0.072393833
0.2	0	0.0197453	0.054798291	0.070322135
0.3	0	0.019505845	0.052735236	0.068268468
0.4	0	0.019267108	0.050689748	0.066232369
0.5	0	0.019029222	0.048661387	0.064213398
0.6	0	0.018792303	0.046649737	0.062211136
0.7	0	0.018556448	0.044654396	0.060225185
0.8	0	0.018321743	0.042674986	0.058255165
0.9	0	0.018088262	0.040711142	0.056300712
1	0	0.017856068	0.038762518	0.054361478
1.1	0	0.017625215	0.03682878	0.052437132
1.2	0	0.017395751	0.03490961	0.050527353
1.3	0	0.017167714	0.033004703	0.048631837
1.4	0	0.016941138	0.031113764	0.04675029
1.5	0	0.016716054	0.029236512	0.04488243
1.6	0	0.016492485	0.027372676	0.043027986
1.7	0	0.016270451	0.025521993	0.041186696
1.8	0	0.016049969	0.023684214	0.039358309
1.9	0	0.015831052	0.021859096	0.037542584
2	0	0.015613712	0.020046404	0.035739285
2.1	0	0.015397957	0.018245914	0.033948188
2.2	0	0.015183791	0.016457406	0.032169074
2.3	0	0.014971221	0.014680672	0.030401733
2.4	0	0.014760248	0.012915506	0.028645961
2.5	0	0.014550872	0.011161712	0.026901561
2.6	0	0.014343094	0.009419099	0.025168342

2.7	0	0.014136912	0.007687482	0.023446119
2.8	0	0.013932323	0.005966682	0.021734713
2.9	0	0.013729323	0.004256525	0.020033951
3	0	0.013527907	0.002556843	0.018343663
3.1	0	0.01332807	0.000867471	0.016663686
3.2	0	0.013129807	-0.000811748	0.014993861
3.3	0	0.012933109	-0.00248097	0.013334034
3.4	0	0.012737971	-0.004140344	0.011684054
3.5	0	0.012544384	-0.005790017	0.010043776
3.6	0	0.01235234	-0.007430129	0.008413058
3.7	0	0.012161831	-0.00906082	0.006791762
3.8	0	0.011972849	-0.010682224	0.005179754
3.9	0	0.011785383	-0.012294471	0.003576901
4	0	0.011599425	-0.013897689	0.001983077
4.1	0	0.011414965	-0.015492003	0.000398158
4.2	0	0.011231994	-0.017077533	-0.001177977
4.3	0	0.011050501	-0.018654399	-0.002745447
4.4	0	0.010870478	-0.020222714	-0.004304368
4.5	0	0.010691913	-0.021782591	-0.005854851
4.6	0	0.010514797	-0.023334141	-0.007397006
4.7	0	0.010339119	-0.02487747	-0.00893094
4.8	0	0.010164869	-0.026412683	-0.010456759
4.9	0	0.009992038	-0.027939883	-0.011974564
5	0	0.009820613	-0.029459169	-0.013484456
5.1	0	0.009650586	-0.030970639	-0.014986532
5.2	0	0.009481946	-0.032474388	-0.016480887
5.3	0	0.009314683	-0.033970511	-0.017967616
5.4	0	0.009148786	-0.035459097	-0.019446809
5.5	0	0.008984245	-0.036940238	-0.020918555
5.6	0	0.00882105	-0.038414019	-0.022382944
5.7	0	0.00865919	-0.039880528	-0.023840059
5.8	0	0.008498657	-0.041339847	-0.025289985

5.9	0	0.008339438	-0.04279206	-0.026732804
6	0	0.008181525	-0.044237245	-0.028168597
6.1	0	0.008024908	-0.045675483	-0.029597442
6.2	0	0.007869576	-0.04710685	-0.031019417
6.3	0	0.00771552	-0.048531423	-0.032434597
6.4	0	0.00756273	-0.049949274	-0.033843057
6.5	0	0.007411197	-0.051360478	-0.035244869
6.6	0	0.00726091	-0.052765106	-0.036640105
6.7	0	0.00711186	-0.054163228	-0.038028835
6.8	0	0.006964038	-0.055554911	-0.039411128
6.9	0	0.006817435	-0.056940225	-0.040787051
7	0	0.00667204	-0.058319235	-0.04215667
7.1	0	0.006527846	-0.059692005	-0.04352005
7.2	0	0.006384842	-0.061058601	-0.044877255
7.3	0	0.00624302	-0.062419084	-0.046228348
7.4	0	0.00610237	-0.063773515	-0.047573391
7.5	0	0.005962885	-0.065121956	-0.048912442
7.6	0	0.005824555	-0.066464466	-0.050245563
7.7	0	0.005687371	-0.067801103	-0.051572811
7.8	0	0.005551325	-0.069131924	-0.052894244
7.9	0	0.005416408	-0.070456986	-0.054209918
8	0	0.005282612	-0.071776344	-0.055519889
8.1	0	0.005149929	-0.073090052	-0.05682421
8.2	0	0.005018349	-0.074398165	-0.058122936
8.3	0	0.004887866	-0.075700734	-0.059416119
8.4	0	0.004758471	-0.076997812	-0.060703811
8.5	0	0.004630156	-0.078289449	-0.061986062
8.6	0	0.004502912	-0.079575696	-0.063262924
8.7	0	0.004376733	-0.080856602	-0.064534445
8.8	0	0.004251611	-0.082132216	-0.065800674
8.9	0	0.004127536	-0.083402585	-0.067061658
9	0	0.004004504	-0.084667756	-0.068317446

9.1	0	0.003882504	-0.085927776	-0.069568082
9.2	0	0.003761531	-0.087182689	-0.070813613
9.3	0	0.003641576	-0.088432542	-0.072054083
9.4	0	0.003522633	-0.089677378	-0.073289538
9.5	0	0.003404695	-0.090917241	-0.074520019
9.6	0	0.003287753	-0.092152174	-0.07574557
9.7	0	0.003171801	-0.093382218	-0.076966234
9.8	0	0.003056833	-0.094607417	-0.078182052
9.9	0	0.002942841	-0.095827809	-0.079393065
10	0	0.002829817	-0.097043437	-0.080599313
10.1	0	0.002717757	-0.098254339	-0.081800837
10.2	0	0.002606652	-0.099460555	-0.082997675
10.3	0	0.002496497	-0.100662124	-0.084189866
10.4	0	0.002387284	-0.101859084	-0.085377449
10.5	0	0.002279008	-0.103051472	-0.08656046
10.6	0	0.002171662	-0.104239326	-0.087738938
10.7	0	0.002065238	-0.105422682	-0.088912919
10.8	0	0.001959733	-0.106601577	-0.090082438
10.9	0	0.001855138	-0.107776045	-0.091247531
11	0	0.001751448	-0.108946122	-0.092408234
11.1	0	0.001648656	-0.110111842	-0.093564581
11.2	0	0.001546758	-0.11127324	-0.094716606
11.3	0	0.001445746	-0.11243035	-0.095864343
11.4	0	0.001345615	-0.113583203	-0.097007825
11.5	0	0.001246359	-0.114731835	-0.098147086
11.6	0	0.001147972	-0.115876276	-0.099282156
11.7	0	0.001050449	-0.117016559	-0.100413069
11.8	0	0.000953784	-0.118152715	-0.101539855
11.9	0	0.000857971	-0.119284775	-0.102662547
12	0	0.000763005	-0.12041277	-0.103781174
12.1	0	0.00066888	-0.121536731	-0.104895768
12.2	0	0.000575592	-0.122656688	-0.106006357

12.3	0	0.000483133	-0.123772669	-0.107112972
12.4	0	0.0003915	-0.124884705	-0.108215642
12.5	0	0.000300687	-0.125992824	-0.109314396
12.6	0	0.000210688	-0.127097054	-0.110409262
12.7	0	0.000121499	-0.128197424	-0.111500268
12.8	0	0.0000331149	-0.129293962	-0.112587443
12.9	0	-0.0000544702	-0.130386695	-0.113670813
13	0	-0.000141261	-0.13147565	-0.114750407
13.1	0	-0.000227262	-0.132560854	-0.11582625
13.2	0	-0.000312478	-0.133642333	-0.116898369
13.3	0	-0.000396915	-0.134720114	-0.11796679
13.4	0	-0.000480577	-0.135794223	-0.11903154
13.5	0	-0.000563469	-0.136864684	-0.120092643
13.6	0	-0.000645595	-0.137931525	-0.121150126
13.7	0	-0.00072696	-0.138994768	-0.122204013
13.8	0	-0.00080757	-0.14005444	-0.123254328
13.9	0	-0.000887428	-0.141110564	-0.124301097
14	0	-0.000966538	-0.142163164	-0.125344343
14.1	0	-0.001044906	-0.143212265	-0.12638409
14.2	0	-0.001122536	-0.144257891	-0.127420362
14.3	0	-0.001199432	-0.145300063	-0.128453182
14.4	0	-0.001275599	-0.146338806	-0.129482573
14.5	0	-0.001351041	-0.147374142	-0.130508558
14.6	0	-0.001425762	-0.148406094	-0.13153116
14.7	0	-0.001499766	-0.149434683	-0.1325504
14.8	0	-0.001573058	-0.150459933	-0.133566302
14.9	0	-0.001645641	-0.151481865	-0.134578886
15	0	-0.001717521	-0.152500501	-0.135588174
15.1	0	-0.0017887	-0.153515861	-0.136594188
15.2	0	-0.001859184	-0.154527967	-0.137596949
15.3	0	-0.001928975	-0.155536841	-0.138596478
15.4	0	-0.001998079	-0.156542501	-0.139592794

15.5	0	-0.002066498	-0.15754497	-0.14058592
15.6	0	-0.002134237	-0.158544267	-0.141575875
15.7	0	-0.0022013	-0.159540412	-0.142562679
15.8	0	-0.00226769	-0.160533426	-0.143546352
15.9	0	-0.002333411	-0.161523327	-0.144526913
16	0	-0.002398467	-0.162510135	-0.145504382
16.1	0	-0.002462862	-0.163493869	-0.146478779
16.2	0	-0.0025266	-0.164474549	-0.147450121
16.3	0	-0.002589683	-0.165452193	-0.148418429
16.4	0	-0.002652116	-0.16642682	-0.14938372
16.5	0	-0.002713902	-0.167398448	-0.150346013
16.6	0	-0.002775045	-0.168367095	-0.151305327
16.7	0	-0.002835548	-0.16933278	-0.152261679
16.8	0	-0.002895415	-0.17029552	-0.153215087
16.9	0	-0.002954649	-0.171255334	-0.15416557
17	0	-0.003013253	-0.172212238	-0.155113144
17.1	0	-0.003071232	-0.17316625	-0.156057827
17.2	0	-0.003128588	-0.174117387	-0.156999636
17.3	0	-0.003185325	-0.175065667	-0.157938588
17.4	0	-0.003241446	-0.176011106	-0.1588747
17.5	0	-0.003296954	-0.176953721	-0.159807989
17.6	0	-0.003351852	-0.177893528	-0.160738472
17.7	0	-0.003406145	-0.178830544	-0.161666164
17.8	0	-0.003459834	-0.179764785	-0.162591082
17.9	0	-0.003512924	-0.180696268	-0.163513242
18	0	-0.003565417	-0.181625007	-0.16443266
18.1	0	-0.003617316	-0.182551019	-0.165349352
18.2	0	-0.003668624	-0.183474319	-0.166263333
18.3	0	-0.003719346	-0.184394923	-0.167174619
18.4	0	-0.003769482	-0.185312847	-0.168083225
18.5	0	-0.003819037	-0.186228104	-0.168989167
18.6	0	-0.003868014	-0.187140712	-0.169892459

18.7	0	-0.003916416	-0.188050684	-0.170793116
18.8	0	-0.003964244	-0.188958034	-0.171691154
18.9	0	-0.004011504	-0.189862779	-0.172586586
19	0	-0.004058196	-0.190764932	-0.173479428
19.1	0	-0.004104324	-0.191664508	-0.174369693
19.2	0	-0.004149892	-0.192561521	-0.175257396
19.3	0	-0.004194901	-0.193455984	-0.176142551
19.4	0	-0.004239355	-0.194347913	-0.177025173
19.5	0	-0.004283255	-0.195237321	-0.177905274
19.6	0	-0.004326607	-0.196124222	-0.178782869
19.7	0	-0.00436941	-0.197008629	-0.179657972
19.8	0	-0.004411669	-0.197890555	-0.180530595
19.9	0	-0.004453387	-0.198770015	-0.181400753
20	0	-0.004494565	-0.199647022	-0.182268458

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1500 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.021583481	0.063358211	0.078720978
0.1	0	0.021332462	0.06125458	0.076626708
0.2	0	0.021081534	0.059169135	0.074550625
0.3	0	0.020830905	0.057101419	0.072492271
0.4	0	0.020580755	0.055050995	0.070451209
0.5	0	0.020331241	0.053017447	0.068427023
0.6	0	0.020082499	0.051000378	0.066419317
0.7	0	0.019834645	0.04899941	0.064427713
0.8	0	0.019587784	0.047014181	0.062451847
0.9	0	0.019342004	0.045044345	0.060491375
1	0	0.019097383	0.04308957	0.058545963
1.1	0	0.018853991	0.041149536	0.056615294

1.2	0	0.018611885	0.03922394	0.054699062
1.3	0	0.018371117	0.037312487	0.052796974
1.4	0	0.018131733	0.035414895	0.050908747
1.5	0	0.017893771	0.033530893	0.04903411
1.6	0	0.017657264	0.031660219	0.047172801
1.7	0	0.01742224	0.029802621	0.045324569
1.8	0	0.017188726	0.027957856	0.04348917
1.9	0	0.016956741	0.02612569	0.04166637
2	0	0.016726303	0.024305896	0.039855942
2.1	0	0.016497427	0.022498255	0.038057667
2.2	0	0.016270124	0.020702555	0.036271334
2.3	0	0.016044405	0.018918592	0.034496738
2.4	0	0.015820276	0.017146168	0.032733681
2.5	0	0.015597744	0.01538509	0.03098197
2.6	0	0.015376812	0.013635173	0.02924142
2.7	0	0.015157483	0.011896236	0.02751185
2.8	0	0.014939757	0.010168104	0.025793085
2.9	0	0.014723635	0.008450607	0.024084956
3	0	0.014509116	0.006743581	0.022387297
3.1	0	0.014296196	0.005046865	0.020699948
3.2	0	0.014084874	0.003360304	0.019022755
3.3	0	0.013875144	0.001683746	0.017355564
3.4	0	0.013667003	0.0000170436	0.01569823
3.5	0	0.013460446	-0.001639945	0.014050608
3.6	0	0.013255465	-0.003287361	0.01241256
3.7	0	0.013052056	-0.004925339	0.01078395
3.8	0	0.012850211	-0.006554011	0.009164646
3.9	0	0.012649922	-0.008173507	0.007554518
4	0	0.012451184	-0.009783951	0.005953441
4.1	0	0.012253987	-0.011385467	0.004361293
4.2	0	0.012058323	-0.012978173	0.002777954
4.3	0	0.011864185	-0.014562187	0.001203308

4.4	0	0.011671563	-0.016137622	-0.000362759
4.5	0	0.011480449	-0.017704588	-0.001920358
4.6	0	0.011290833	-0.019263196	-0.003469597
4.7	0	0.011102707	-0.020813549	-0.005010584
4.8	0	0.010916061	-0.022355753	-0.00654342
4.9	0	0.010730887	-0.023889907	-0.008068207
5	0	0.010547173	-0.025416111	-0.009585044
5.1	0	0.010364912	-0.026934462	-0.011094028
5.2	0	0.010184093	-0.028445055	-0.012595253
5.3	0	0.010004708	-0.029947981	-0.014088812
5.4	0	0.009826746	-0.031443331	-0.015574796
5.5	0	0.009650197	-0.032931194	-0.017053293
5.6	0	0.009475052	-0.034411658	-0.01852439
5.7	0	0.009301301	-0.035884806	-0.019988171
5.8	0	0.009128936	-0.037350722	-0.021444721
5.9	0	0.008957945	-0.038809487	-0.022894121
6	0	0.00878832	-0.040261183	-0.02433645
6.1	0	0.00862005	-0.041705886	-0.025771787
6.2	0	0.008453127	-0.043143673	-0.02720021
6.3	0	0.008287541	-0.044574621	-0.028621792
6.4	0	0.008123282	-0.045998802	-0.030036608
6.5	0	0.007960341	-0.04741629	-0.031444731
6.6	0	0.007798708	-0.048827155	-0.032846231
6.7	0	0.007638375	-0.050231467	-0.034241179
6.8	0	0.007479332	-0.051629294	-0.035629642
6.9	0	0.007321569	-0.053020704	-0.037011688
7	0	0.007165078	-0.054405762	-0.038387382
7.1	0	0.007009849	-0.055784534	-0.03975679
7.2	0	0.006855874	-0.057157082	-0.041119976
7.3	0	0.006703143	-0.05852347	-0.042477
7.4	0	0.006551648	-0.059883758	-0.043827926
7.5	0	0.00640138	-0.061238008	-0.045172813

7.6	0	0.006252329	-0.062586277	-0.04651172
7.7	0	0.006104489	-0.063928625	-0.047844706
7.8	0	0.005957849	-0.065265108	-0.049171828
7.9	0	0.005812401	-0.066595783	-0.050493141
8	0	0.005668137	-0.067920705	-0.051808703
8.1	0	0.005525048	-0.069239929	-0.053118566
8.2	0	0.005383127	-0.070553507	-0.054422784
8.3	0	0.005242365	-0.071861494	-0.055721411
8.4	0	0.005102753	-0.073163939	-0.057014497
8.5	0	0.004964284	-0.074460896	-0.058302094
8.6	0	0.004826949	-0.075752412	-0.059584252
8.7	0	0.004690742	-0.077038539	-0.060861019
8.8	0	0.004555653	-0.078319323	-0.062132446
8.9	0	0.004421675	-0.079594814	-0.063398579
9	0	0.004288801	-0.080865058	-0.064659466
9.1	0	0.004157022	-0.082130102	-0.065915152
9.2	0	0.004026332	-0.08338999	-0.067165684
9.3	0	0.003896722	-0.084644769	-0.068411107
9.4	0	0.003768185	-0.085894482	-0.069651464
9.5	0	0.003640715	-0.087139173	-0.0708868
9.6	0	0.003514303	-0.088378885	-0.072117157
9.7	0	0.003388942	-0.08961366	-0.073342578
9.8	0	0.003264626	-0.09084354	-0.074563104
9.9	0	0.003141347	-0.092068566	-0.075778776
10	0	0.003019098	-0.093288778	-0.076989635
10.1	0	0.002897873	-0.094504217	-0.078195721
10.2	0	0.002777664	-0.095714922	-0.079397074
10.3	0	0.002658465	-0.096920931	-0.080593731
10.4	0	0.002540268	-0.098122283	-0.081785732
10.5	0	0.002423068	-0.099319015	-0.082973113
10.6	0	0.002306858	-0.100511166	-0.084155913
10.7	0	0.002191631	-0.101698771	-0.085334168

10.8	0	0.002077381	-0.102881866	-0.086507914
10.9	0	0.001964101	-0.104060487	-0.087677187
11	0	0.001851785	-0.105234671	-0.088842022
11.1	0	0.001740427	-0.10640445	-0.090002453
11.2	0	0.00163002	-0.10756986	-0.091158516
11.3	0	0.001520558	-0.108730934	-0.092310243
11.4	0	0.001412036	-0.109887706	-0.093457669
11.5	0	0.001304448	-0.111040209	-0.094600826
11.6	0	0.001197786	-0.112188475	-0.095739747
11.7	0	0.001092046	-0.113332536	-0.096874464
11.8	0	0.000987222	-0.114472425	-0.098005008
11.9	0	0.000883307	-0.115608171	-0.099131411
12	0	0.000780296	-0.116739807	-0.100253704
12.1	0	0.000678183	-0.117867362	-0.101371917
12.2	0	0.000576964	-0.118990868	-0.102486081
12.3	0	0.000476631	-0.120110352	-0.103596224
12.4	0	0.00037718	-0.121225846	-0.104702377
12.5	0	0.000278605	-0.122337378	-0.105804569
12.6	0	0.000180901	-0.123444976	-0.106902828
12.7	0	0.0000840627	-0.124548669	-0.107997182
12.8	0	-0.000011916	-0.125648485	-0.10908766
12.9	0	-0.00010704	-0.126744451	-0.110174288
13	0	-0.000201314	-0.127836595	-0.111257096
13.1	0	-0.000294743	-0.128924944	-0.112336108
13.2	0	-0.000387334	-0.130009524	-0.113411353
13.3	0	-0.00047909	-0.131090362	-0.114482856
13.4	0	-0.000570016	-0.132167484	-0.115550643
13.5	0	-0.000660119	-0.133240915	-0.11661474
13.6	0	-0.000749402	-0.134310681	-0.117675174
13.7	0	-0.00083787	-0.135376807	-0.118731967
13.8	0	-0.000925529	-0.136439318	-0.119785147
13.9	0	-0.001012382	-0.137498239	-0.120834736

14	0	-0.001098436	-0.138553593	-0.12188076
14.1	0	-0.001183694	-0.139605405	-0.122923243
14.2	0	-0.001268161	-0.140653699	-0.123962207
14.3	0	-0.001351841	-0.141698498	-0.124997678
14.4	0	-0.00143474	-0.142739825	-0.126029677
14.5	0	-0.001516862	-0.143777703	-0.127058228
14.6	0	-0.001598211	-0.144812155	-0.128083354
14.7	0	-0.001678792	-0.145843203	-0.129105077
14.8	0	-0.001758608	-0.14687087	-0.130123419
14.9	0	-0.001837665	-0.147895178	-0.131138403
15	0	-0.001915967	-0.148916148	-0.132150049
15.1	0	-0.001993518	-0.149933802	-0.13315838
15.2	0	-0.002070322	-0.15094816	-0.134163417
15.3	0	-0.002146384	-0.151959245	-0.135165181
15.4	0	-0.002221707	-0.152967077	-0.136163693
15.5	0	-0.002296296	-0.153971677	-0.137158973
15.6	0	-0.002370155	-0.154973064	-0.138151041
15.7	0	-0.002443288	-0.15597126	-0.139139919
15.8	0	-0.002515698	-0.156966284	-0.140125625
15.9	0	-0.00258739	-0.157958156	-0.141108181
16	0	-0.002658368	-0.158946895	-0.142087604
16.1	0	-0.002728636	-0.159932521	-0.143063915
16.2	0	-0.002798197	-0.160915053	-0.144037133
16.3	0	-0.002867056	-0.161894511	-0.145007277
16.4	0	-0.002935216	-0.162870911	-0.145974365
16.5	0	-0.003002681	-0.163844275	-0.146938416
16.6	0	-0.003069455	-0.164814619	-0.147899449
16.7	0	-0.003135541	-0.165781962	-0.148857482
16.8	0	-0.003200943	-0.166746322	-0.149812533
16.9	0	-0.003265665	-0.167707717	-0.150764619
17	0	-0.00332971	-0.168666165	-0.151713759
17.1	0	-0.003393082	-0.169621683	-0.15265997

17.2	0	-0.003455784	-0.170574288	-0.153603269
17.3	0	-0.003517821	-0.171523998	-0.154543674
17.4	0	-0.003579195	-0.17247083	-0.155481201
17.5	0	-0.00363991	-0.1734148	-0.156415868
17.6	0	-0.003699969	-0.174355926	-0.157347691
17.7	0	-0.003759376	-0.175294223	-0.158276686
17.8	0	-0.003818135	-0.176229708	-0.15920287
17.9	0	-0.003876247	-0.177162398	-0.16012626
18	0	-0.003933718	-0.178092308	-0.161046871
18.1	0	-0.00399055	-0.179019455	-0.161964719
18.2	0	-0.004046745	-0.179943854	-0.16287982
18.3	0	-0.004102309	-0.18086552	-0.16379219
18.4	0	-0.004157243	-0.18178447	-0.164701843
18.5	0	-0.004211552	-0.182700718	-0.165608797
18.6	0	-0.004265237	-0.18361428	-0.166513065
18.7	0	-0.004318303	-0.184525171	-0.167414662
18.8	0	-0.004370752	-0.185433406	-0.168313605
18.9	0	-0.004422587	-0.186338999	-0.169209906
19	0	-0.004473812	-0.187241965	-0.170103582
19.1	0	-0.004524429	-0.188142319	-0.170994647
19.2	0	-0.004574443	-0.189040075	-0.171883114
19.3	0	-0.004623854	-0.189935248	-0.172768999
19.4	0	-0.004672667	-0.190827851	-0.173652315
19.5	0	-0.004720884	-0.191717898	-0.174533076
19.6	0	-0.004768509	-0.192605404	-0.175411298
19.7	0	-0.004815544	-0.193490382	-0.176286992
19.8	0	-0.004861992	-0.194372846	-0.177160172
19.9	0	-0.004907856	-0.19525281	-0.178030854
20	0	-0.004953138	-0.196130285	-0.178899048

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1600 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.022956347	0.067687362	0.082901936
0.1	0	0.02269531	0.06558049	0.080804386
0.2	0	0.022434056	0.063491454	0.078724671
0.3	0	0.02217282	0.061419821	0.07666236
0.4	0	0.021911805	0.059365182	0.074617044
0.5	0	0.021651191	0.057327146	0.072588331
0.6	0	0.021391135	0.055305337	0.070575846
0.7	0	0.021131773	0.053299397	0.068579231
0.8	0	0.020873225	0.051308984	0.066598143
0.9	0	0.020615599	0.049333767	0.064632252
1	0	0.020358985	0.047373431	0.062681242
1.1	0	0.020103468	0.045427672	0.060744809
1.2	0	0.019849118	0.043496199	0.058822663
1.3	0	0.019595999	0.04157873	0.056914522
1.4	0	0.019344167	0.039674996	0.055020115
1.5	0	0.019093671	0.037784735	0.053139183
1.6	0	0.018844553	0.035907696	0.051271473
1.7	0	0.018596852	0.034043637	0.049416743
1.8	0	0.018350601	0.032192324	0.047574759
1.9	0	0.018105827	0.03035353	0.045745296
2	0	0.017862556	0.028527037	0.043928133
2.1	0	0.01762081	0.026712632	0.042123059
2.2	0	0.017380605	0.024910111	0.04032987
2.3	0	0.017141958	0.023119276	0.038548366
2.4	0	0.016904882	0.021339935	0.036778356
2.5	0	0.016669388	0.0195719	0.035019653
2.6	0	0.016435483	0.017814991	0.033272077

2.7	0	0.016203177	0.016069032	0.031535451
2.8	0	0.015972472	0.014333854	0.029809606
2.9	0	0.015743374	0.01260929	0.028094376
3	0	0.015515885	0.01089518	0.026389599
3.1	0	0.015290006	0.009191368	0.024695121
3.2	0	0.015065737	0.007497701	0.023010788
3.3	0	0.014843077	0.005814031	0.021336453
3.4	0	0.014622025	0.004140215	0.019671972
3.5	0	0.014402579	0.002476112	0.018017204
3.6	0	0.014184734	0.000821586	0.016372014
3.7	0	0.013968487	-0.000823496	0.014736267
3.8	0	0.013753834	-0.002459264	0.013109834
3.9	0	0.013540769	-0.004085845	0.011492589
4	0	0.013329287	-0.005703362	0.009884408
4.1	0	0.013119382	-0.007311935	0.008285172
4.2	0	0.012911047	-0.008911681	0.006694762
4.3	0	0.012704276	-0.010502715	0.005113064
4.4	0	0.012499062	-0.01208515	0.003539966
4.5	0	0.012295397	-0.013659094	0.001975359
4.6	0	0.012093274	-0.015224655	0.000419135
4.7	0	0.011892685	-0.016781936	-0.001128809
4.8	0	0.011693622	-0.01833104	-0.002668576
4.9	0	0.011496077	-0.019872067	-0.004200265
5	0	0.011300041	-0.021405114	-0.005723975
5.1	0	0.011105506	-0.022930277	-0.007239801
5.2	0	0.010912463	-0.02444765	-0.008747836
5.3	0	0.010720904	-0.025957323	-0.010248171
5.4	0	0.01053082	-0.027459386	-0.011740897
5.5	0	0.010342202	-0.028953928	-0.013226101
5.6	0	0.01015504	-0.030441034	-0.014703869
5.7	0	0.009969327	-0.031920787	-0.016174285
5.8	0	0.009785053	-0.033393272	-0.017637432

5.9	0	0.00960221	-0.034858568	-0.01909339
6	0	0.009420787	-0.036316754	-0.020542239
6.1	0	0.009240776	-0.037767909	-0.021984056
6.2	0	0.009062168	-0.039212108	-0.023418917
6.3	0	0.008884953	-0.040649427	-0.024846898
6.4	0	0.008709124	-0.042079938	-0.026268072
6.5	0	0.00853467	-0.043503714	-0.027682509
6.6	0	0.008361583	-0.044920824	-0.029090282
6.7	0	0.008189854	-0.046331339	-0.03049146
6.8	0	0.008019473	-0.047735326	-0.031886109
6.9	0	0.007850432	-0.049132852	-0.033274298
7	0	0.007682722	-0.050523983	-0.034656091
7.1	0	0.007516334	-0.051908782	-0.036031553
7.2	0	0.007351259	-0.053287314	-0.037400748
7.3	0	0.007187489	-0.05465964	-0.038763737
7.4	0	0.007025015	-0.056025822	-0.040120582
7.5	0	0.006863827	-0.057385919	-0.041471343
7.6	0	0.006703918	-0.058739991	-0.042816077
7.7	0	0.006545279	-0.060088095	-0.044154845
7.8	0	0.006387902	-0.061430289	-0.045487702
7.9	0	0.006231778	-0.062766628	-0.046814705
8	0	0.006076898	-0.064097168	-0.048135909
8.1	0	0.005923254	-0.065421963	-0.049451368
8.2	0	0.005770838	-0.066741066	-0.050761136
8.3	0	0.005619643	-0.06805453	-0.052065264
8.4	0	0.005469659	-0.069362406	-0.053363805
8.5	0	0.005320878	-0.070664746	-0.05465681
8.6	0	0.005173294	-0.071961599	-0.055944328
8.7	0	0.005026897	-0.073253015	-0.057226409
8.8	0	0.004881679	-0.074539041	-0.058503102
8.9	0	0.004737634	-0.075819727	-0.059774453
9	0	0.004594753	-0.077095118	-0.06104051

9.1	0	0.004453029	-0.078365262	-0.06230132
9.2	0	0.004312453	-0.079630203	-0.063556928
9.3	0	0.004173019	-0.080889987	-0.064807379
9.4	0	0.004034718	-0.082144658	-0.066052717
9.5	0	0.003897545	-0.083394259	-0.067292986
9.6	0	0.00376149	-0.084638834	-0.068528228
9.7	0	0.003626547	-0.085878425	-0.069758486
9.8	0	0.003492709	-0.087113073	-0.070983803
9.9	0	0.003359968	-0.088342819	-0.072204218
10	0	0.003228317	-0.089567705	-0.073419773
10.1	0	0.00309775	-0.09078777	-0.074630507
10.2	0	0.002968259	-0.092003054	-0.07583646
10.3	0	0.002839837	-0.093213594	-0.077037671
10.4	0	0.002712478	-0.094419431	-0.078234177
10.5	0	0.002586175	-0.095620601	-0.079426018
10.6	0	0.002460921	-0.096817142	-0.08061323
10.7	0	0.002336709	-0.09800909	-0.081795849
10.8	0	0.002213533	-0.099196482	-0.082973913
10.9	0	0.002091386	-0.100379354	-0.084147456
11	0	0.001970263	-0.10155774	-0.085316515
11.1	0	0.001850155	-0.102731676	-0.086481124
11.2	0	0.001731057	-0.103901196	-0.087641318
11.3	0	0.001612963	-0.105066334	-0.088797129
11.4	0	0.001495867	-0.106227124	-0.089948593
11.5	0	0.001379762	-0.107383598	-0.091095741
11.6	0	0.001264642	-0.108535789	-0.092238607
11.7	0	0.001150501	-0.109683729	-0.093377223
11.8	0	0.001037333	-0.110827451	-0.09451162
11.9	0	0.000925132	-0.111966985	-0.09564183
12	0	0.000813893	-0.113102362	-0.096767884
12.1	0	0.000703609	-0.114233614	-0.097889813
12.2	0	0.000594274	-0.11536077	-0.099007647

12.3	0	0.000485883	-0.11648386	-0.100121415
12.4	0	0.00037843	-0.117602914	-0.101231147
12.5	0	0.00027191	-0.118717961	-0.102336873
12.6	0	0.000166317	-0.119829029	-0.103438621
12.7	0	0.0000616446	-0.120936147	-0.104536419
12.8	0	-0.0000421115	-0.122039344	-0.105630296
12.9	0	-0.000144957	-0.123138646	-0.10672028
13	0	-0.000246898	-0.124234082	-0.107806397
13.1	0	-0.000347939	-0.125325678	-0.108888675
13.2	0	-0.000448086	-0.126413462	-0.109967141
13.3	0	-0.000547343	-0.127497459	-0.111041821
13.4	0	-0.000645716	-0.128577696	-0.112112742
13.5	0	-0.000743211	-0.129654198	-0.113179929
13.6	0	-0.000839832	-0.130726992	-0.114243407
13.7	0	-0.000935584	-0.131796103	-0.115303203
13.8	0	-0.001030472	-0.132861555	-0.116359341
13.9	0	-0.001124502	-0.133923373	-0.117411846
14	0	-0.001217677	-0.134981582	-0.118460742
14.1	0	-0.001310004	-0.136036206	-0.119506053
14.2	0	-0.001401487	-0.137087269	-0.120547804
14.3	0	-0.00149213	-0.138134794	-0.121586018
14.4	0	-0.001581939	-0.139178804	-0.122620718
14.5	0	-0.001670918	-0.140219324	-0.123651927
14.6	0	-0.001759072	-0.141256375	-0.124679669
14.7	0	-0.001846405	-0.14228998	-0.125703965
14.8	0	-0.001932922	-0.143320162	-0.126724839
14.9	0	-0.002018627	-0.144346943	-0.127742312
15	0	-0.002103526	-0.145370345	-0.128756407
15.1	0	-0.002187622	-0.146390389	-0.129767145
15.2	0	-0.00227092	-0.147407096	-0.130774546
15.3	0	-0.002353424	-0.148420488	-0.131778634
15.4	0	-0.002435138	-0.149430587	-0.132779428

15.5	0	-0.002516068	-0.150437412	-0.133776949
15.6	0	-0.002596217	-0.151440984	-0.134771218
15.7	0	-0.002675589	-0.152441324	-0.135762256
15.8	0	-0.002754189	-0.153438451	-0.136750081
15.9	0	-0.00283202	-0.154432386	-0.137734715
16	0	-0.002909088	-0.155423148	-0.138716177
16.1	0	-0.002985395	-0.156410757	-0.139694486
16.2	0	-0.003060946	-0.157395232	-0.140669662
16.3	0	-0.003135746	-0.158376592	-0.141641724
16.4	0	-0.003209797	-0.159354856	-0.142610691
16.5	0	-0.003283104	-0.160330044	-0.143576581
16.6	0	-0.003355671	-0.161302172	-0.144539414
16.7	0	-0.003427502	-0.162271261	-0.145499207
16.8	0	-0.003498601	-0.163237327	-0.146455979
16.9	0	-0.003568971	-0.164200389	-0.147409747
17	0	-0.003638616	-0.165160466	-0.14836053
17.1	0	-0.00370754	-0.166117573	-0.149308345
17.2	0	-0.003775747	-0.16707173	-0.15025321
17.3	0	-0.00384324	-0.168022953	-0.151195142
17.4	0	-0.003910024	-0.168971259	-0.152134159
17.5	0	-0.003976101	-0.169916666	-0.153070276
17.6	0	-0.004041475	-0.17085919	-0.154003511
17.7	0	-0.00410615	-0.171798848	-0.154933882
17.8	0	-0.00417013	-0.172735656	-0.155861403
17.9	0	-0.004233417	-0.173669632	-0.156786092
18	0	-0.004296016	-0.17460079	-0.157707965
18.1	0	-0.00435793	-0.175529148	-0.158627038
18.2	0	-0.004419162	-0.17645472	-0.159543326
18.3	0	-0.004479715	-0.177377523	-0.160456846
18.4	0	-0.004539594	-0.178297573	-0.161367614
18.5	0	-0.004598801	-0.179214884	-0.162275644
18.6	0	-0.00465734	-0.180129473	-0.163180952

18.7	0	-0.004715214	-0.181041354	-0.164083553
18.8	0	-0.004772426	-0.181950542	-0.164983462
18.9	0	-0.00482898	-0.182857053	-0.165880695
19	0	-0.004884879	-0.183760901	-0.166775265
19.1	0	-0.004940125	-0.184662101	-0.167667188
19.2	0	-0.004994723	-0.185560667	-0.168556479
19.3	0	-0.005048675	-0.186456614	-0.169443151
19.4	0	-0.005101984	-0.187349955	-0.170327218
19.5	0	-0.005154654	-0.188240706	-0.171208696
19.6	0	-0.005206687	-0.18912888	-0.172087598
19.7	0	-0.005258087	-0.190014491	-0.172963938
19.8	0	-0.005308857	-0.190897553	-0.173837729
19.9	0	-0.005358999	-0.191778079	-0.174708986
20	0	-0.005408517	-0.192656084	-0.175577721

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1700 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.024341992	0.071960768	0.087027379
0.1	0	0.024071448	0.069851327	0.084927259
0.2	0	0.023800375	0.067759361	0.082844615
0.3	0	0.023529034	0.065684468	0.080779045
0.4	0	0.023257652	0.063626263	0.078730164
0.5	0	0.02298643	0.061584376	0.076697602
0.6	0	0.022715544	0.059558454	0.074681007
0.7	0	0.022445149	0.057548159	0.072680039
0.8	0	0.022175383	0.055553166	0.070694375
0.9	0	0.021906366	0.053573161	0.0687237
1	0	0.021638208	0.051607846	0.066767715
1.1	0	0.021371002	0.04965693	0.064826131

1.2	0	0.021104835	0.047720136	0.062898669
1.3	0	0.02083978	0.045797195	0.060985062
1.4	0	0.020575905	0.043887848	0.05908505
1.5	0	0.020313269	0.041991847	0.057198384
1.6	0	0.020051925	0.040108949	0.055324823
1.7	0	0.019791918	0.038238923	0.053464134
1.8	0	0.019533291	0.036381542	0.051616091
1.9	0	0.019276078	0.034536589	0.049780477
2	0	0.019020314	0.032703853	0.047957081
2.1	0	0.018766025	0.030883129	0.046145698
2.2	0	0.018513236	0.02907422	0.04434613
2.3	0	0.018261969	0.027276934	0.042558187
2.4	0	0.018012242	0.025491084	0.04078168
2.5	0	0.017764073	0.023716491	0.03901643
2.6	0	0.017517473	0.021952977	0.037262262
2.7	0	0.017272455	0.020200374	0.035519004
2.8	0	0.017029028	0.018458515	0.033786492
2.9	0	0.016787201	0.01672724	0.032064563
3	0	0.01654698	0.015006391	0.030353063
3.1	0	0.01630837	0.013295818	0.028651837
3.2	0	0.016071374	0.01159537	0.026960739
3.3	0	0.015835995	0.009904905	0.025279624
3.4	0	0.015602234	0.008224281	0.02360835
3.5	0	0.015370092	0.006553362	0.021946782
3.6	0	0.015139568	0.004892014	0.020294785
3.7	0	0.014910661	0.003240106	0.01865223
3.8	0	0.014683368	0.001597512	0.017018989
3.9	0	0.014457687	-0.0000358914	0.015394939
4	0	0.014233615	-0.001660226	0.013779958
4.1	0	0.014011147	-0.00327561	0.012173929
4.2	0	0.013790279	-0.004882158	0.010576736
4.3	0	0.013571007	-0.006479984	0.008988266

4.4	0	0.013353324	-0.008069196	0.00740841
4.5	0	0.013137226	-0.009649902	0.005837061
4.6	0	0.012922706	-0.011222208	0.004274112
4.7	0	0.012709758	-0.012786216	0.002719461
4.8	0	0.012498374	-0.014342026	0.001173009
4.9	0	0.012288549	-0.015889738	-0.000365344
5	0	0.012080276	-0.017429447	-0.001895695
5.1	0	0.011873546	-0.018961248	-0.003418136
5.2	0	0.011668352	-0.020485233	-0.004932761
5.3	0	0.011464687	-0.022001491	-0.006439659
5.4	0	0.011262543	-0.023510112	-0.007938919
5.5	0	0.011061911	-0.025011181	-0.009430628
5.6	0	0.010862784	-0.026504785	-0.01091487
5.7	0	0.010665155	-0.027991005	-0.012391729
5.8	0	0.010469013	-0.029469925	-0.013861287
5.9	0	0.010274351	-0.030941623	-0.015323622
6	0	0.010081162	-0.032406178	-0.016778815
6.1	0	0.009889435	-0.033863666	-0.01822694
6.2	0	0.009699163	-0.035314164	-0.019668075
6.3	0	0.009510338	-0.036757746	-0.021102293
6.4	0	0.009322295	-0.038194483	-0.022529667
6.5	0	0.009136992	-0.039624448	-0.023950268
6.6	0	0.008952454	-0.04104771	-0.025364165
6.7	0	0.008769328	-0.042464337	-0.026771429
6.8	0	0.008587606	-0.043874398	-0.028172125
6.9	0	0.008407279	-0.045277959	-0.029566321
7	0	0.008228338	-0.046675084	-0.030954082
7.1	0	0.008050775	-0.048065839	-0.032335471
7.2	0	0.007874582	-0.049450284	-0.033710552
7.3	0	0.007699749	-0.050828483	-0.035079385
7.4	0	0.007526269	-0.052200496	-0.036442033
7.5	0	0.007354133	-0.053566383	-0.037798554

7.6	0	0.007183332	-0.054926202	-0.039149008
7.7	0	0.007013859	-0.056280011	-0.040493451
7.8	0	0.006845705	-0.057627867	-0.041831941
7.9	0	0.006678861	-0.058969826	-0.043164534
8	0	0.00651332	-0.060305942	-0.044491284
8.1	0	0.006349073	-0.06163627	-0.045812245
8.2	0	0.006186112	-0.062960862	-0.047127471
8.3	0	0.006024429	-0.064279771	-0.048437014
8.4	0	0.005864016	-0.065593049	-0.049740926
8.5	0	0.005704865	-0.066900745	-0.051039256
8.6	0	0.005546968	-0.068202911	-0.052332056
8.7	0	0.005390317	-0.069499595	-0.053619374
8.8	0	0.005234905	-0.070790845	-0.054901258
8.9	0	0.005080723	-0.072076709	-0.056177756
9	0	0.004927763	-0.073357235	-0.057448915
9.1	0	0.004776019	-0.074632467	-0.058714782
9.2	0	0.004625482	-0.075902452	-0.059975401
9.3	0	0.004476146	-0.077167235	-0.061230818
9.4	0	0.004328001	-0.078426859	-0.062481077
9.5	0	0.004181042	-0.079681369	-0.063726221
9.6	0	0.00403526	-0.080930807	-0.064966293
9.7	0	0.003890648	-0.082175215	-0.066201336
9.8	0	0.0037472	-0.083414636	-0.067431391
9.9	0	0.003604907	-0.084649109	-0.0686565
10	0	0.003463763	-0.085878677	-0.069876703
10.1	0	0.00332376	-0.087103378	-0.071092039
10.2	0	0.003184892	-0.088323252	-0.072302549
10.3	0	0.003047151	-0.089538339	-0.073508271
10.4	0	0.002910531	-0.090748675	-0.074709243
10.5	0	0.002775025	-0.0919543	-0.075905504
10.6	0	0.002640625	-0.09315525	-0.07709709
10.7	0	0.002507325	-0.094351563	-0.078284039

10.8	0	0.002375119	-0.095543274	-0.079466387
10.9	0	0.002244	-0.096730419	-0.080644169
11	0	0.002113961	-0.097913033	-0.081817421
11.1	0	0.001984996	-0.099091152	-0.082986177
11.2	0	0.001857097	-0.100264811	-0.084150473
11.3	0	0.00173026	-0.101434042	-0.085310342
11.4	0	0.001604477	-0.102598879	-0.086465818
11.5	0	0.001479742	-0.103759356	-0.087616934
11.6	0	0.001356049	-0.104915505	-0.088763722
11.7	0	0.001233391	-0.106067359	-0.089906215
11.8	0	0.001111764	-0.10721495	-0.091044445
11.9	0	0.000991159	-0.108358308	-0.092178443
12	0	0.000871572	-0.109497465	-0.09330824
12.1	0	0.000752996	-0.110632451	-0.094433867
12.2	0	0.000635426	-0.111763298	-0.095555355
12.3	0	0.000518855	-0.112890034	-0.096672733
12.4	0	0.000403278	-0.11401269	-0.09778603
12.5	0	0.000288689	-0.115131295	-0.098895277
12.6	0	0.000175082	-0.116245877	-0.100000502
12.7	0	0.0000624519	-0.117356465	-0.101101733
12.8	0	-0.0000492076	-0.118463088	-0.102198999
12.9	0	-0.000159902	-0.119565772	-0.103292328
13	0	-0.000269636	-0.120664547	-0.104381747
13.1	0	-0.000378417	-0.121759438	-0.105467283
13.2	0	-0.000486248	-0.122850473	-0.106548963
13.3	0	-0.000593136	-0.123937679	-0.107626814
13.4	0	-0.000699086	-0.125021081	-0.108700862
13.5	0	-0.000804103	-0.126100706	-0.109771134
13.6	0	-0.000908192	-0.127176579	-0.110837654
13.7	0	-0.001011359	-0.128248725	-0.111900449
13.8	0	-0.001111361	-0.129317171	-0.112959542
13.9	0	-0.001214948	-0.13038194	-0.11401496

14	0	-0.001315379	-0.131443057	-0.115066727
14.1	0	-0.001414908	-0.132500547	-0.116114866
14.2	0	-0.001513541	-0.133554433	-0.117159403
14.3	0	-0.001611281	-0.13460474	-0.11820036
14.4	0	-0.001708135	-0.13565149	-0.119237761
14.5	0	-0.001804106	-0.136694706	-0.12027163
14.6	0	-0.0018992	-0.137734413	-0.121301989
14.7	0	-0.001993421	-0.138770633	-0.122328862
14.8	0	-0.002086774	-0.139803387	-0.12335227
14.9	0	-0.002179265	-0.140832699	-0.124372236
15	0	-0.002270897	-0.14185859	-0.125388782
15.1	0	-0.002361675	-0.142881082	-0.12640193
15.2	0	-0.002451603	-0.143900197	-0.127411701
15.3	0	-0.002540688	-0.144915956	-0.128418117
15.4	0	-0.002628932	-0.145928379	-0.129421198
15.5	0	-0.00271634	-0.146937489	-0.130420966
15.6	0	-0.002802917	-0.147943306	-0.131417442
15.7	0	-0.002888667	-0.148945849	-0.132410645
15.8	0	-0.002973594	-0.14994514	-0.133400596
15.9	0	-0.003057703	-0.150941198	-0.134387315
16	0	-0.003140999	-0.151934044	-0.135370822
16.1	0	-0.003223484	-0.152923696	-0.136351136
16.2	0	-0.003305165	-0.153910174	-0.137328278
16.3	0	-0.003386044	-0.154893499	-0.138302266
16.4	0	-0.003466126	-0.155873687	-0.139273119
16.5	0	-0.003545414	-0.156850759	-0.140240856
16.6	0	-0.003623915	-0.157824734	-0.141205496
16.7	0	-0.00370163	-0.158795628	-0.142167057
16.8	0	-0.003778564	-0.159763462	-0.143125559
16.9	0	-0.003854721	-0.160728253	-0.144081018
17	0	-0.003930106	-0.161690019	-0.145033453
17.1	0	-0.004004721	-0.162648778	-0.145982881

17.2	0	-0.004078572	-0.163604547	-0.146929321
17.3	0	-0.004151661	-0.164557344	-0.147872789
17.4	0	-0.004223992	-0.165507186	-0.148813303
17.5	0	-0.004295571	-0.166454091	-0.149750881
17.6	0	-0.004366399	-0.167398075	-0.150685538
17.7	0	-0.004436481	-0.168339155	-0.151617293
17.8	0	-0.00450582	-0.169277348	-0.152546161
17.9	0	-0.004574421	-0.170212669	-0.153472159
18	0	-0.004642287	-0.171145137	-0.154395303
18.1	0	-0.004709421	-0.172074766	-0.15531561
18.2	0	-0.004775828	-0.173001573	-0.156233096
18.3	0	-0.00484151	-0.173925573	-0.157147776
18.4	0	-0.004906471	-0.174846783	-0.158059666
18.5	0	-0.004970715	-0.175765218	-0.158968782
18.6	0	-0.005034245	-0.176680893	-0.159875139
18.7	0	-0.005097065	-0.177593824	-0.160778753
18.8	0	-0.005159178	-0.178504026	-0.161679639
18.9	0	-0.005220587	-0.179411514	-0.162577812
19	0	-0.005281296	-0.180316303	-0.163473287
19.1	0	-0.005341309	-0.181218408	-0.164366078
19.2	0	-0.005400627	-0.182117843	-0.1652562
19.3	0	-0.005459256	-0.183014622	-0.166143669
19.4	0	-0.005517198	-0.183908761	-0.167028497
19.5	0	-0.005574456	-0.184800274	-0.1679107
19.6	0	-0.005631033	-0.185689174	-0.168790291
19.7	0	-0.005686933	-0.186575475	-0.169667285
19.8	0	-0.00574216	-0.187459192	-0.170541696
19.9	0	-0.005796715	-0.188340339	-0.171413536
20	0	-0.005850602	-0.189218929	-0.172282821

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1800 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.025744004	0.076175721	0.091099904
0.1	0	0.025464569	0.074064511	0.088997978
0.2	0	0.025184279	0.071970401	0.086913153
0.3	0	0.024903418	0.069893015	0.084845053
0.4	0	0.024622237	0.067831993	0.082793317
0.5	0	0.024340958	0.065786988	0.0807576
0.6	0	0.024059775	0.063757669	0.078737568
0.7	0	0.023778863	0.061743715	0.076732903
0.8	0	0.023498375	0.05974482	0.074743298
0.9	0	0.023218449	0.057760689	0.072768456
1	0	0.022939208	0.055791036	0.070808095
1.1	0	0.02266076	0.053835588	0.068861938
1.2	0	0.022383202	0.05189408	0.066929722
1.3	0	0.022106622	0.049966257	0.065011192
1.4	0	0.021831098	0.048051871	0.063106099
1.5	0	0.021556699	0.046150685	0.061214207
1.6	0	0.021283488	0.044262467	0.059335284
1.7	0	0.021011152	0.042386996	0.057469107
1.8	0	0.020740846	0.040524054	0.055615461
1.9	0	0.020471509	0.038673433	0.053774137
2	0	0.020203548	0.036834929	0.05194493
2.1	0	0.019937001	0.035008348	0.050127646
2.2	0	0.019671897	0.033193496	0.048322092
2.3	0	0.019408265	0.03139019	0.046528085
2.4	0	0.019146129	0.029598251	0.044745444
2.5	0	0.018885512	0.027817502	0.042973995
2.6	0	0.018626431	0.026047775	0.041213568

2.7	0	0.018368904	0.024288904	0.039463997
2.8	0	0.018112945	0.022540729	0.037725124
2.9	0	0.017858566	0.020803095	0.035996791
3	0	0.017605778	0.019075849	0.034278846
3.1	0	0.017354591	0.017358842	0.032571142
3.2	0	0.017105011	0.015651932	0.030873534
3.3	0	0.016857044	0.013954977	0.029185882
3.4	0	0.016610695	0.01226784	0.027508049
3.5	0	0.016365968	0.010590389	0.025839901
3.6	0	0.016122865	0.008922493	0.024181309
3.7	0	0.015881388	0.007264024	0.022532145
3.8	0	0.015641537	0.005614859	0.020892285
3.9	0	0.015403312	0.003974877	0.019261608
4	0	0.015166712	0.00234396	0.017639996
4.1	0	0.014931736	0.000721991	0.016027334
4.2	0	0.014698381	-0.000891141	0.014423508
4.3	0	0.014466644	-0.002495547	0.012828408
4.4	0	0.014236522	-0.004091336	0.011241926
4.5	0	0.014008012	-0.005678611	0.009663958
4.6	0	0.013781108	-0.007257477	0.008094399
4.7	0	0.013555807	-0.008828034	0.00653315
4.8	0	0.013332103	-0.010390381	0.00498011
4.9	0	0.01310999	-0.011944615	0.003435184
5	0	0.012889464	-0.01349083	0.001898278
5.1	0	0.012670518	-0.015029119	0.000369297
5.2	0	0.012453145	-0.016559573	-0.001151848
5.3	0	0.01223734	-0.01808228	-0.002665246
5.4	0	0.012023096	-0.019597328	-0.004170985
5.5	0	0.011810406	-0.021104801	-0.005669149
5.6	0	0.011599262	-0.022604785	-0.007159824
5.7	0	0.011389658	-0.02409736	-0.008643089
5.8	0	0.011181587	-0.025582608	-0.010119027

5.9	0	0.01097504	-0.027060606	-0.011587715
6	0	0.010770011	-0.028531433	-0.013049233
6.1	0	0.010566491	-0.029995165	-0.014503654
6.2	0	0.010364474	-0.031451875	-0.015951054
6.3	0	0.01016395	-0.032901638	-0.017391507
6.4	0	0.009964913	-0.034344525	-0.018825083
6.5	0	0.009767355	-0.035780606	-0.020251854
6.6	0	0.009571267	-0.037209951	-0.021671889
6.7	0	0.009376641	-0.038632628	-0.023085255
6.8	0	0.00918347	-0.040048704	-0.02449202
6.9	0	0.008991745	-0.041458244	-0.025892249
7	0	0.008801458	-0.042861312	-0.027286007
7.1	0	0.008612602	-0.044257973	-0.028673358
7.2	0	0.008425167	-0.045648288	-0.030054362
7.3	0	0.008239147	-0.04703232	-0.031429083
7.4	0	0.008054532	-0.048410127	-0.032797579
7.5	0	0.007871316	-0.049781769	-0.034159911
7.6	0	0.007689488	-0.051147305	-0.035516136
7.7	0	0.007509043	-0.052506792	-0.036866312
7.8	0	0.007329972	-0.053860285	-0.038210495
7.9	0	0.007152266	-0.055207842	-0.039548741
8	0	0.006975917	-0.056549515	-0.040881104
8.1	0	0.006800918	-0.057885359	-0.042207637
8.2	0	0.006627261	-0.059215427	-0.043528395
8.3	0	0.006454938	-0.060539771	-0.044843428
8.4	0	0.00628394	-0.061858441	-0.046152788
8.5	0	0.006114261	-0.063171489	-0.047456526
8.6	0	0.005945892	-0.064478963	-0.04875469
8.7	0	0.005778826	-0.065780913	-0.050047331
8.8	0	0.005613054	-0.067077388	-0.051334496
8.9	0	0.00544857	-0.068368434	-0.052616232
9	0	0.005285365	-0.069654098	-0.053892586

9.1	0	0.005123432	-0.070934426	-0.055163605
9.2	0	0.004962763	-0.072209464	-0.056429334
9.3	0	0.004803352	-0.073479255	-0.057689816
9.4	0	0.004645189	-0.074743845	-0.058945098
9.5	0	0.004488269	-0.076003277	-0.060195221
9.6	0	0.004332584	-0.077257593	-0.061440229
9.7	0	0.004178125	-0.078506837	-0.062680164
9.8	0	0.004024887	-0.079751048	-0.063915067
9.9	0	0.003872862	-0.080990268	-0.06514498
10	0	0.003722043	-0.082224539	-0.066369942
10.1	0	0.003572422	-0.083453899	-0.067589995
10.2	0	0.003423993	-0.084678388	-0.068805177
10.3	0	0.003276748	-0.085898045	-0.070015527
10.4	0	0.003130681	-0.087112907	-0.071221083
10.5	0	0.002985785	-0.088323014	-0.072421883
10.6	0	0.002842052	-0.089528402	-0.073617965
10.7	0	0.002699477	-0.090729108	-0.074809365
10.8	0	0.002558052	-0.091925167	-0.075996119
10.9	0	0.002417771	-0.093116617	-0.077178264
11	0	0.002278626	-0.094303492	-0.078355834
11.1	0	0.002140612	-0.095485827	-0.079528864
11.2	0	0.002003722	-0.096663657	-0.08069739
11.3	0	0.00186795	-0.097837016	-0.081861444
11.4	0	0.001733288	-0.099005936	-0.083021061
11.5	0	0.00159973	-0.100170452	-0.084176274
11.6	0	0.001467271	-0.101330596	-0.085327114
11.7	0	0.001335904	-0.1024864	-0.086473616
11.8	0	0.001205622	-0.103637896	-0.08761581
11.9	0	0.00107642	-0.104785116	-0.088753728
12	0	0.000948291	-0.105928091	-0.089887401
12.1	0	0.00082123	-0.107066851	-0.09101686
12.2	0	0.000695229	-0.108201428	-0.092142136

12.3	0	0.000570284	-0.10933185	-0.093263258
12.4	0	0.000446388	-0.110458148	-0.094380256
12.5	0	0.000323536	-0.11158035	-0.095493159
12.6	0	0.00020172	-0.112698487	-0.096601996
12.7	0	0.0000809369	-0.113812586	-0.097706796
12.8	0	-0.0000388207	-0.114922676	-0.098807587
12.9	0	-0.000157558	-0.116028784	-0.099904398
13	0	-0.000275281	-0.117130938	-0.100997255
13.1	0	-0.000391995	-0.118229166	-0.102086186
13.2	0	-0.000507705	-0.119323494	-0.103171217
13.3	0	-0.000622418	-0.12041395	-0.104252377
13.4	0	-0.000736138	-0.121500559	-0.10532969
13.5	0	-0.000848871	-0.122583347	-0.106403184
13.6	0	-0.000960623	-0.123662341	-0.107472883
13.7	0	-0.001071399	-0.124737566	-0.108538813
13.8	0	-0.001181203	-0.125809046	-0.109601
13.9	0	-0.001290042	-0.126876808	-0.110659468
14	0	-0.001397921	-0.127940874	-0.111714242
14.1	0	-0.001504844	-0.129001271	-0.112765347
14.2	0	-0.001610818	-0.130058022	-0.113812806
14.3	0	-0.001715846	-0.131111151	-0.114856644
14.4	0	-0.001819935	-0.132160681	-0.115896883
14.5	0	-0.001923088	-0.133206636	-0.116933548
14.6	0	-0.002025312	-0.134249039	-0.117966661
14.7	0	-0.00212661	-0.135287912	-0.118996246
14.8	0	-0.002226989	-0.136323278	-0.120022324
14.9	0	-0.002326452	-0.137355161	-0.121044918
15	0	-0.002425004	-0.13838358	-0.122064051
15.1	0	-0.002522651	-0.13940856	-0.123079744
15.2	0	-0.002619397	-0.140430121	-0.124092018
15.3	0	-0.002715247	-0.141448284	-0.125100896
15.4	0	-0.002810205	-0.142463071	-0.126106398

15.5	0	-0.002904276	-0.143474504	-0.127108546
15.6	0	-0.002997464	-0.144482601	-0.128107361
15.7	0	-0.003089775	-0.145487385	-0.129102862
15.8	0	-0.003181212	-0.146488876	-0.13009507
15.9	0	-0.003271781	-0.147487094	-0.131084005
16	0	-0.003361485	-0.148482058	-0.132069688
16.1	0	-0.003450329	-0.149473788	-0.133052138
16.2	0	-0.003538318	-0.150462305	-0.134031375
16.3	0	-0.003625455	-0.151447627	-0.135007417
16.4	0	-0.003711745	-0.152429773	-0.135980285
16.5	0	-0.003797192	-0.153408763	-0.136949997
16.6	0	-0.003881801	-0.154384615	-0.137916572
16.7	0	-0.003965575	-0.155357349	-0.138880029
16.8	0	-0.00404852	-0.156326981	-0.139840385
16.9	0	-0.004130638	-0.157293531	-0.14079766
17	0	-0.004211934	-0.158257017	-0.141751871
17.1	0	-0.004292413	-0.159217457	-0.142703037
17.2	0	-0.004372077	-0.160174868	-0.143651175
17.3	0	-0.004450932	-0.161129267	-0.144596302
17.4	0	-0.004528982	-0.162080673	-0.145538436
17.5	0	-0.004606229	-0.163029103	-0.146477594
17.6	0	-0.004682678	-0.163974573	-0.147413794
17.7	0	-0.004758333	-0.164917101	-0.148347052
17.8	0	-0.004833198	-0.165856703	-0.149277385
17.9	0	-0.004907277	-0.166793396	-0.15020481
18	0	-0.004980573	-0.167727196	-0.151129343
18.1	0	-0.00505309	-0.16865812	-0.152051
18.2	0	-0.005124832	-0.169586184	-0.152969798
18.3	0	-0.005195803	-0.170511403	-0.153885752
18.4	0	-0.005266006	-0.171433795	-0.154798879
18.5	0	-0.005335445	-0.172353373	-0.155709194
18.6	0	-0.005404124	-0.173270155	-0.156616713

18.7	0	-0.005472046	-0.174184155	-0.157521451
18.8	0	-0.005539215	-0.175095389	-0.158423423
18.9	0	-0.005605634	-0.176003871	-0.159322645
19	0	-0.005671306	-0.176909618	-0.160219132
19.1	0	-0.005736237	-0.177812643	-0.161112898
19.2	0	-0.005800427	-0.178712962	-0.162003959
19.3	0	-0.005863883	-0.179610589	-0.162892329
19.4	0	-0.005926606	-0.180505539	-0.163778022
19.5	0	-0.0059886	-0.181397826	-0.164661053
19.6	0	-0.006049868	-0.182287464	-0.165541437
19.7	0	-0.006110414	-0.183174468	-0.166419186
19.8	0	-0.006170241	-0.184058851	-0.167294316
19.9	0	-0.006229353	-0.184940627	-0.16816684
20	0	-0.006287752	-0.185819811	-0.169036772

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 1900 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.027151974	0.080336469	0.095111895
0.1	0	0.026864004	0.078224085	0.093008744
0.2	0	0.026574858	0.07612843	0.090922324
0.3	0	0.026284841	0.074049152	0.088852282
0.4	0	0.025994228	0.071985912	0.08679828
0.5	0	0.025703257	0.069938388	0.084759994
0.6	0	0.025412144	0.067906266	0.082737111
0.7	0	0.025121079	0.065889245	0.080729331
0.8	0	0.024830233	0.063887036	0.078736364
0.9	0	0.024539757	0.061899359	0.07675793
1	0	0.024249787	0.059925945	0.07479376
1.1	0	0.023960446	0.057966533	0.072843594

1.2	0	0.023671843	0.056020873	0.07090718
1.3	0	0.023384077	0.05408872	0.068984275
1.4	0	0.023097238	0.052169841	0.067074644
1.5	0	0.022811403	0.050264008	0.06517806
1.6	0	0.022526646	0.048371	0.063294303
1.7	0	0.022243031	0.046490603	0.061423158
1.8	0	0.021960616	0.044622612	0.059564419
1.9	0	0.021679454	0.042766826	0.057717886
2	0	0.021399591	0.040923049	0.055883364
2.1	0	0.02112107	0.039091093	0.054060663
2.2	0	0.020843929	0.037270775	0.052249601
2.3	0	0.020568203	0.035461916	0.050449999
2.4	0	0.020293921	0.033664342	0.048661684
2.5	0	0.020021111	0.031877886	0.046884487
2.6	0	0.019749798	0.030102384	0.045118244
2.7	0	0.019480003	0.028337676	0.043362797
2.8	0	0.019211745	0.026583606	0.041617989
2.9	0	0.018945042	0.024840024	0.039883669
3	0	0.018679907	0.023106782	0.038159691
3.1	0	0.018416354	0.021383737	0.036445909
3.2	0	0.018154395	0.019670749	0.034742186
3.3	0	0.017894038	0.017967681	0.033048383
3.4	0	0.017635293	0.0162744	0.031364369
3.5	0	0.017378165	0.014590776	0.029690012
3.6	0	0.017122661	0.012916682	0.028025187
3.7	0	0.016868784	0.011251996	0.026369769
3.8	0	0.016616539	0.009596595	0.024723637
3.9	0	0.016365928	0.007950362	0.023086674
4	0	0.016116952	0.006313181	0.021458763
4.1	0	0.015869612	0.004684939	0.019839793
4.2	0	0.015623909	0.003065526	0.018229652
4.3	0	0.01537984	0.001454835	0.016628234

4.4	0	0.015137406	-0.000147241	0.015035431
4.5	0	0.014896605	-0.001740804	0.013451142
4.6	0	0.014657433	-0.003325955	0.011875265
4.7	0	0.014419888	-0.004902794	0.010307701
4.8	0	0.014183967	-0.006471418	0.008748354
4.9	0	0.013949665	-0.00803192	0.007197128
5	0	0.013716979	-0.009584394	0.005653931
5.1	0	0.013485904	-0.011128931	0.004118671
5.2	0	0.013256436	-0.012665621	0.00259126
5.3	0	0.013028568	-0.014194549	0.00107161
5.4	0	0.012802297	-0.015715803	-0.000440365
5.5	0	0.012577615	-0.017229466	-0.001944749
5.6	0	0.012354517	-0.018735621	-0.003441623
5.7	0	0.012132997	-0.020234348	-0.004931069
5.8	0	0.011913049	-0.021725726	-0.006413167
5.9	0	0.011694666	-0.023209834	-0.007887993
6	0	0.011477842	-0.024686747	-0.009355625
6.1	0	0.01126257	-0.026156542	-0.010816137
6.2	0	0.011048842	-0.02761929	-0.012269602
6.3	0	0.010836653	-0.029075065	-0.013716094
6.4	0	0.010625994	-0.030523937	-0.015155682
6.5	0	0.010416859	-0.031965976	-0.016588438
6.6	0	0.01020924	-0.033401251	-0.018014428
6.7	0	0.01000313	-0.034829828	-0.019433721
6.8	0	0.009798522	-0.036251774	-0.020846382
6.9	0	0.009595408	-0.037667154	-0.022252476
7	0	0.00939378	-0.039076032	-0.023652068
7.1	0	0.009193631	-0.04047847	-0.025045219
7.2	0	0.008994953	-0.041874529	-0.026431993
7.3	0	0.00879774	-0.043264272	-0.027812448
7.4	0	0.008601982	-0.044647756	-0.029186646
7.5	0	0.008407672	-0.046025042	-0.030554644

7.6	0	0.008214804	-0.047396187	-0.031916501
7.7	0	0.008023368	-0.048761247	-0.033272274
7.8	0	0.007833357	-0.050120278	-0.034622017
7.9	0	0.007644765	-0.051473336	-0.035965787
8	0	0.007457582	-0.052820475	-0.037303637
8.1	0	0.007271801	-0.054161748	-0.038635621
8.2	0	0.007087415	-0.055497207	-0.039961791
8.3	0	0.006904416	-0.056826904	-0.041282198
8.4	0	0.006722796	-0.05815089	-0.042596895
8.5	0	0.006542547	-0.059469215	-0.04390593
8.6	0	0.006363663	-0.060781928	-0.045209354
8.7	0	0.006186135	-0.062089078	-0.046507215
8.8	0	0.006009957	-0.063390714	-0.04779956
8.9	0	0.005835119	-0.064686881	-0.049086437
9	0	0.005661616	-0.065977627	-0.050367892
9.1	0	0.005489439	-0.067262996	-0.051643972
9.2	0	0.005318581	-0.068543036	-0.052914721
9.3	0	0.005149035	-0.06981779	-0.054180183
9.4	0	0.004980793	-0.071087301	-0.055440404
9.5	0	0.004813849	-0.072351613	-0.056695426
9.6	0	0.004648194	-0.073610769	-0.057945291
9.7	0	0.004483821	-0.074864811	-0.059190042
9.8	0	0.004320724	-0.07611378	-0.06042972
9.9	0	0.004158895	-0.077357717	-0.061664366
10	0	0.003998327	-0.078596663	-0.06289402
10.1	0	0.003839014	-0.079830656	-0.064118722
10.2	0	0.003680947	-0.081059738	-0.065338512
10.3	0	0.00352412	-0.082283945	-0.066553428
10.4	0	0.003368526	-0.083503316	-0.067763509
10.5	0	0.003214159	-0.08471789	-0.068968791
10.6	0	0.00306101	-0.085927702	-0.070169313
10.7	0	0.002909074	-0.087132791	-0.07136511

10.8	0	0.002758344	-0.088333191	-0.072556219
10.9	0	0.002608813	-0.08952894	-0.073742677
11	0	0.002460475	-0.090720071	-0.074924517
11.1	0	0.002313322	-0.091906621	-0.076101776
11.2	0	0.002167348	-0.093088623	-0.077274487
11.3	0	0.002022547	-0.094266111	-0.078442685
11.4	0	0.001878912	-0.095439119	-0.079606402
11.5	0	0.001736437	-0.09660768	-0.080765673
11.6	0	0.001595115	-0.097771827	-0.081920529
11.7	0	0.00145494	-0.098931591	-0.083071003
11.8	0	0.001315906	-0.100087006	-0.084217128
11.9	0	0.001178006	-0.101238102	-0.085358934
12	0	0.001041234	-0.102384911	-0.086496452
12.1	0	0.000905584	-0.103527462	-0.087629714
12.2	0	0.000771051	-0.104665788	-0.08875875
12.3	0	0.000637627	-0.105799917	-0.08988359
12.4	0	0.000505307	-0.106929879	-0.091004263
12.5	0	0.000374084	-0.108055704	-0.092120799
12.6	0	0.000243954	-0.109177421	-0.093233227
12.7	0	0.00011491	-0.110295058	-0.094341575
12.8	0	-0.0000130545	-0.111408643	-0.095445872
12.9	0	-0.000139944	-0.112518205	-0.096546146
13	0	-0.000265766	-0.113623772	-0.097642424
13.1	0	-0.000390524	-0.114725369	-0.098734734
13.2	0	-0.000514225	-0.115823025	-0.099823102
13.3	0	-0.000636875	-0.116916767	-0.100907556
13.4	0	-0.000758479	-0.11800662	-0.101988122
13.5	0	-0.000879042	-0.119092611	-0.103064826
13.6	0	-0.00099857	-0.120174765	-0.104137694
13.7	0	-0.001117069	-0.121253108	-0.105206752
13.8	0	-0.001234544	-0.122327666	-0.106272024
13.9	0	-0.001351	-0.123398464	-0.107333535

14	0	-0.001466443	-0.124465525	-0.108391311
14.1	0	-0.001580878	-0.125528875	-0.109445376
14.2	0	-0.00169431	-0.126588537	-0.110495754
14.3	0	-0.001806745	-0.127644536	-0.111542468
14.4	0	-0.001918187	-0.128696896	-0.112585544
14.5	0	-0.002028642	-0.129745639	-0.113625003
14.6	0	-0.002138115	-0.130790788	-0.114660869
14.7	0	-0.002246611	-0.131832368	-0.115693166
14.8	0	-0.002354134	-0.1328704	-0.116721915
14.9	0	-0.002460691	-0.133904906	-0.11774714
15	0	-0.002566285	-0.13493591	-0.118768861
15.1	0	-0.002670922	-0.135963433	-0.119787103
15.2	0	-0.002774607	-0.136987496	-0.120801885
15.3	0	-0.002877344	-0.138008122	-0.12181323
15.4	0	-0.002979139	-0.139025331	-0.122821159
15.5	0	-0.003079995	-0.140039145	-0.123825693
15.6	0	-0.003179918	-0.141049584	-0.124826853
15.7	0	-0.003278913	-0.14205667	-0.125824659
15.8	0	-0.003376983	-0.143060422	-0.126819133
15.9	0	-0.003474135	-0.144060861	-0.127810294
16	0	-0.003570371	-0.145058007	-0.128798162
16.1	0	-0.003665697	-0.14605188	-0.129782757
16.2	0	-0.003760118	-0.147042498	-0.1307641
16.3	0	-0.003853637	-0.148029883	-0.131742208
16.4	0	-0.003946259	-0.149014053	-0.132717102
16.5	0	-0.004037989	-0.149995028	-0.133688801
16.6	0	-0.004128831	-0.150972825	-0.134657324
16.7	0	-0.00421879	-0.151947464	-0.135622688
16.8	0	-0.004307869	-0.152918963	-0.136584914
16.9	0	-0.004396072	-0.153887342	-0.137544019
17	0	-0.004483405	-0.154852617	-0.138500021
17.1	0	-0.004569872	-0.155814806	-0.139452939

17.2	0	-0.004655475	-0.156773929	-0.14040279
17.3	0	-0.004740221	-0.157730002	-0.141349591
17.4	0	-0.004824112	-0.158683043	-0.142293362
17.5	0	-0.004907154	-0.159633069	-0.143234118
17.6	0	-0.004989349	-0.160580098	-0.144171877
17.7	0	-0.005070702	-0.161524146	-0.145106656
17.8	0	-0.005151217	-0.16246523	-0.146038471
17.9	0	-0.005230897	-0.163403367	-0.146967341
18	0	-0.005309748	-0.164338574	-0.147893281
18.1	0	-0.005387773	-0.165270867	-0.148816307
18.2	0	-0.005464975	-0.166200262	-0.149736436
18.3	0	-0.005541359	-0.167126776	-0.150653684
18.4	0	-0.005616928	-0.168050424	-0.151568067
18.5	0	-0.005691686	-0.168971221	-0.1524796
18.6	0	-0.005765637	-0.169889185	-0.1533883
18.7	0	-0.005838784	-0.17080433	-0.154294182
18.8	0	-0.005911132	-0.171716672	-0.155197262
18.9	0	-0.005982684	-0.172626226	-0.156097554
19	0	-0.006053444	-0.173533007	-0.156995074
19.1	0	-0.006123415	-0.17443703	-0.157889836
19.2	0	-0.006192601	-0.17533831	-0.158781857
19.3	0	-0.006261005	-0.176236862	-0.159671149
19.4	0	-0.006328632	-0.1771327	-0.160557729
19.5	0	-0.006395484	-0.178025839	-0.161441611
19.6	0	-0.006461565	-0.178916294	-0.162322808
19.7	0	-0.006526878	-0.179804078	-0.163201335
19.8	0	-0.006591428	-0.180689205	-0.164077207
19.9	0	-0.006655217	-0.18157169	-0.164950437
20	0	-0.006718249	-0.182451546	-0.165821039

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2000 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.028560974	0.084437635	0.099068993
0.1	0	0.028264942	0.082324661	0.096965215
0.2	0	0.02796742	0.080228047	0.094877797
0.3	0	0.027668738	0.078147464	0.092806412
0.4	0	0.027369185	0.076082596	0.090750742
0.5	0	0.027069021	0.074033138	0.088710484
0.6	0	0.026768477	0.071998796	0.086685344
0.7	0	0.026467758	0.069979288	0.084675038
0.8	0	0.02616705	0.067974339	0.082679293
0.9	0	0.02586652	0.065983687	0.080697845
1	0	0.025566315	0.064007076	0.078730439
1.1	0	0.025266571	0.062044259	0.076776829
1.2	0	0.024967408	0.060094998	0.074836775
1.3	0	0.024668937	0.058159061	0.072910047
1.4	0	0.024371256	0.056236225	0.070996421
1.5	0	0.024074455	0.054326274	0.06909568
1.6	0	0.023778614	0.052428996	0.067207614
1.7	0	0.023483807	0.050544188	0.065332019
1.8	0	0.023190101	0.048671652	0.063468697
1.9	0	0.022897555	0.046811197	0.061617456
2	0	0.022606223	0.044962634	0.059778109
2.1	0	0.022316155	0.043125784	0.057950475
2.2	0	0.022027396	0.041300469	0.056134378
2.3	0	0.021739986	0.039486518	0.054329646
2.4	0	0.021453961	0.037683765	0.052536112
2.5	0	0.021169354	0.035892047	0.050753613
2.6	0	0.020886194	0.034111205	0.048981993

2.7	0	0.020604509	0.032341087	0.047221096
2.8	0	0.020324323	0.030581541	0.045470773
2.9	0	0.020045656	0.028832422	0.043730877
3	0	0.019768528	0.027093587	0.042001267
3.1	0	0.019492956	0.025364897	0.040281802
3.2	0	0.019218955	0.023646216	0.038572347
3.3	0	0.018946538	0.021937412	0.036872769
3.4	0	0.018675717	0.020238356	0.03518294
3.5	0	0.018406502	0.018548921	0.033502734
3.6	0	0.018138903	0.016868984	0.031832026
3.7	0	0.017872925	0.015198425	0.030170696
3.8	0	0.017608576	0.013537126	0.028518627
3.9	0	0.017345861	0.011884972	0.026875704
4	0	0.017084784	0.01024185	0.025241814
4.1	0	0.016825349	0.008607651	0.023616847
4.2	0	0.016567557	0.006982267	0.022000696
4.3	0	0.01631141	0.005365592	0.020393254
4.4	0	0.016056909	0.003757523	0.01879442
4.5	0	0.015804055	0.002157959	0.017204091
4.6	0	0.015552847	0.000566802	0.015622169
4.7	0	0.015303283	-0.001016045	0.014048558
4.8	0	0.015055362	-0.002590677	0.012483163
4.9	0	0.014809083	-0.004157187	0.01092589
5	0	0.014564442	-0.005715666	0.009376649
5.1	0	0.014321436	-0.007266204	0.00783535
5.2	0	0.014080063	-0.008808887	0.006301906
5.3	0	0.013840318	-0.010343801	0.004776231
5.4	0	0.013602197	-0.011871031	0.003258241
5.5	0	0.013365697	-0.013390659	0.001747853
5.6	0	0.013130811	-0.014902767	0.000244987
5.7	0	0.012897536	-0.016407433	-0.001250438
5.8	0	0.012665866	-0.017904735	-0.002738498

5.9	0	0.012435796	-0.019394751	-0.004219271
6	0	0.012207321	-0.020877554	-0.005692832
6.1	0	0.011980433	-0.02235322	-0.007159255
6.2	0	0.011755128	-0.023821821	-0.008618611
6.3	0	0.011531399	-0.025283426	-0.010070973
6.4	0	0.01130924	-0.026738108	-0.01151641
6.5	0	0.011088644	-0.028185934	-0.012954991
6.6	0	0.010869606	-0.029626972	-0.014386783
6.7	0	0.010652118	-0.031061288	-0.015811854
6.8	0	0.010436173	-0.032488948	-0.017230268
6.9	0	0.010221766	-0.033910015	-0.018642088
7	0	0.010008888	-0.035324553	-0.02004738
7.1	0	0.009797533	-0.036732624	-0.021446203
7.2	0	0.009587695	-0.038134288	-0.02283862
7.3	0	0.009379365	-0.039529607	-0.024224691
7.4	0	0.009172536	-0.040918638	-0.025604474
7.5	0	0.008967203	-0.04230144	-0.026978027
7.6	0	0.008763356	-0.04367807	-0.028345408
7.7	0	0.00856099	-0.045048584	-0.029706673
7.8	0	0.008360096	-0.046413038	-0.031061878
7.9	0	0.008160668	-0.047771486	-0.032411077
8	0	0.007962698	-0.049123981	-0.033754323
8.1	0	0.007766179	-0.050470578	-0.035091669
8.2	0	0.007571103	-0.051811327	-0.036423168
8.3	0	0.007377464	-0.05314628	-0.03774887
8.4	0	0.007185253	-0.054475487	-0.039068827
8.5	0	0.006994464	-0.055798998	-0.040383087
8.6	0	0.006805089	-0.057116863	-0.041691701
8.7	0	0.006617121	-0.058429128	-0.042994715
8.8	0	0.006430552	-0.059735843	-0.044292178
8.9	0	0.006245376	-0.061037053	-0.045584137
9	0	0.006061584	-0.062332805	-0.046870638

9.1	0	0.005879171	-0.063623145	-0.048151725
9.2	0	0.005698128	-0.064908117	-0.049427445
9.3	0	0.005518448	-0.066187765	-0.050697841
9.4	0	0.005340124	-0.067462133	-0.051962958
9.5	0	0.00516315	-0.068731265	-0.053222837
9.6	0	0.004987516	-0.069995202	-0.054477522
9.7	0	0.004813218	-0.071253987	-0.055727054
9.8	0	0.004640248	-0.07250766	-0.056971475
9.9	0	0.004468598	-0.073756262	-0.058210824
10	0	0.004298261	-0.074999835	-0.059445144
10.1	0	0.004129231	-0.076238416	-0.060674472
10.2	0	0.003961501	-0.077472045	-0.061898849
10.3	0	0.003795063	-0.078700761	-0.063118312
10.4	0	0.003629911	-0.079924602	-0.0643329
10.5	0	0.003466038	-0.081143605	-0.065542651
10.6	0	0.003303438	-0.082357808	-0.0667476
10.7	0	0.003142103	-0.083567247	-0.067947786
10.8	0	0.002982026	-0.084771957	-0.069143244
10.9	0	0.002823202	-0.085971976	-0.07033401
11	0	0.002665623	-0.087167337	-0.071520118
11.1	0	0.002509283	-0.088358076	-0.072701605
11.2	0	0.002354175	-0.089544228	-0.073878503
11.3	0	0.002200293	-0.090725825	-0.075050848
11.4	0	0.002047629	-0.091902902	-0.076218672
11.5	0	0.001896179	-0.093075491	-0.077382008
11.6	0	0.001745935	-0.094243625	-0.07854089
11.7	0	0.001596891	-0.095407336	-0.079695349
11.8	0	0.00144904	-0.096566657	-0.080845418
11.9	0	0.001302377	-0.097721619	-0.081991127
12	0	0.001156895	-0.098872252	-0.083132508
12.1	0	0.001012588	-0.100018588	-0.084269592
12.2	0	0.00086945	-0.101160657	-0.085402409

12.3	0	0.000727474	-0.102298488	-0.086530989
12.4	0	0.000586655	-0.103432113	-0.087655362
12.5	0	0.000446987	-0.104561559	-0.088775557
12.6	0	0.000308463	-0.105686856	-0.089891603
12.7	0	0.000171077	-0.106808032	-0.091003528
12.8	0	0.0000348245	-0.107925116	-0.092111361
12.9	0	-0.000100301	-0.109038137	-0.093215131
13	0	-0.000234306	-0.11014712	-0.094314864
13.1	0	-0.000367196	-0.111252094	-0.095410587
13.2	0	-0.000498976	-0.112353086	-0.096502329
13.3	0	-0.000629653	-0.113450123	-0.097590116
13.4	0	-0.000759231	-0.11454323	-0.098673974
13.5	0	-0.000887717	-0.115632435	-0.099753929
13.6	0	-0.001015117	-0.116717762	-0.100830007
13.7	0	-0.001141435	-0.117799239	-0.101902234
13.8	0	-0.001266677	-0.118876889	-0.102970636
13.9	0	-0.001390848	-0.119950738	-0.104035236
14	0	-0.001513955	-0.12102081	-0.10509606
14.1	0	-0.001636003	-0.122087131	-0.106153133
14.2	0	-0.001756996	-0.123149724	-0.107206479
14.3	0	-0.00187694	-0.124208613	-0.10825612
14.4	0	-0.00199584	-0.125263822	-0.109302083
14.5	0	-0.002113703	-0.126315375	-0.110344389
14.6	0	-0.002230532	-0.127363295	-0.111383061
14.7	0	-0.002346333	-0.128407603	-0.112418124
14.8	0	-0.002461111	-0.129448325	-0.1134496
14.9	0	-0.002574872	-0.130485481	-0.114477511
15	0	-0.00268762	-0.131519095	-0.115501879
15.1	0	-0.00279936	-0.132549187	-0.116522727
15.2	0	-0.002910097	-0.133575781	-0.117540076
15.3	0	-0.003019836	-0.134598897	-0.118553947
15.4	0	-0.003128583	-0.135618557	-0.119564364

15.5	0	-0.003236341	-0.136634782	-0.120571345
15.6	0	-0.003343116	-0.137647593	-0.121574913
15.7	0	-0.003448913	-0.138657011	-0.122575088
15.8	0	-0.003553736	-0.139663056	-0.123571891
15.9	0	-0.003657591	-0.140665748	-0.124565342
16	0	-0.00376048	-0.141665109	-0.125555461
16.1	0	-0.003862411	-0.142661157	-0.126542268
16.2	0	-0.003963386	-0.143653912	-0.127525782
16.3	0	-0.004063411	-0.144643394	-0.128506025
16.4	0	-0.004162491	-0.145629623	-0.129483013
16.5	0	-0.004260628	-0.146612617	-0.130456768
16.6	0	-0.00435783	-0.147592395	-0.131427307
16.7	0	-0.004454099	-0.148568977	-0.13239465
16.8	0	-0.004549439	-0.14954238	-0.133358816
16.9	0	-0.004643857	-0.150512624	-0.134319822
17	0	-0.004737355	-0.151479726	-0.135277687
17.1	0	-0.004829939	-0.152443704	-0.136232429
17.2	0	-0.004921612	-0.153404577	-0.137184066
17.3	0	-0.005012379	-0.154362363	-0.138132615
17.4	0	-0.005102243	-0.155317078	-0.139078096
17.5	0	-0.00519121	-0.156268741	-0.140020524
17.6	0	-0.005279284	-0.157217368	-0.140959917
17.7	0	-0.005366468	-0.158162977	-0.141896292
17.8	0	-0.005452766	-0.159105585	-0.142829666
17.9	0	-0.005538184	-0.160045208	-0.143760057
18	0	-0.005622724	-0.160981863	-0.14468748
18.1	0	-0.005706391	-0.161915566	-0.145611952
18.2	0	-0.005789189	-0.162846335	-0.146533489
18.3	0	-0.005871122	-0.163774185	-0.147452109
18.4	0	-0.005952193	-0.164699132	-0.148367826
18.5	0	-0.006032407	-0.165621192	-0.149280656
18.6	0	-0.006111768	-0.166540381	-0.150190617

18.7	0	-0.00619028	-0.167456714	-0.151097722
18.8	0	-0.006267945	-0.168370207	-0.152001988
18.9	0	-0.006344769	-0.169280876	-0.152903429
19	0	-0.006420755	-0.170188736	-0.153802062
19.1	0	-0.006495906	-0.171093801	-0.154697902
19.2	0	-0.006570227	-0.171996087	-0.155590962
19.3	0	-0.00664372	-0.172895608	-0.156481259
19.4	0	-0.006716391	-0.173792379	-0.157368806
19.5	0	-0.006788242	-0.174686416	-0.158253619
19.6	0	-0.006859277	-0.175577731	-0.159135712
19.7	0	-0.0069295	-0.17646634	-0.160015099
19.8	0	-0.006998914	-0.177352257	-0.160891794
19.9	0	-0.007067523	-0.178235496	-0.161765812
20	0	-0.00713533	-0.179116071	-0.162637166

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2100 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.029985965	0.088488008	0.102970207
0.1	0	0.029682474	0.086375144	0.100866521
0.2	0	0.029377169	0.084278262	0.098778818
0.3	0	0.029070398	0.082197055	0.096706792
0.4	0	0.028762471	0.080131228	0.094650147
0.5	0	0.028453664	0.078080495	0.092608598
0.6	0	0.028144224	0.076044582	0.090581869
0.7	0	0.027834373	0.074023221	0.088569695
0.8	0	0.027524312	0.072016157	0.086571817
0.9	0	0.027214219	0.070023139	0.084587988
1	0	0.026904258	0.068043927	0.082617967
1.1	0	0.026594574	0.066078288	0.080661519

1.2	0	0.026285301	0.064125995	0.078718419
1.3	0	0.02597656	0.062186831	0.076788449
1.4	0	0.025668458	0.060260581	0.074871395
1.5	0	0.025361096	0.058347041	0.072967051
1.6	0	0.025054564	0.05644601	0.071075218
1.7	0	0.024748945	0.054557294	0.0691957
1.8	0	0.024444311	0.052680703	0.06732831
1.9	0	0.024140733	0.050816054	0.065472862
2	0	0.02383827	0.04896317	0.06362918
2.1	0	0.023536981	0.047121875	0.061797089
2.2	0	0.023236916	0.045292001	0.059976419
2.3	0	0.022938121	0.043473384	0.058167008
2.4	0	0.02264064	0.041665863	0.056368694
2.5	0	0.022344511	0.039869283	0.054581322
2.6	0	0.022049769	0.03808349	0.052804738
2.7	0	0.021756446	0.036308338	0.051038796
2.8	0	0.02146457	0.03454368	0.049283349
2.9	0	0.021174169	0.032789377	0.047538258
3	0	0.020885265	0.03104529	0.045803384
3.1	0	0.020597881	0.029311285	0.044078593
3.2	0	0.020312034	0.027587231	0.042363754
3.3	0	0.020027743	0.025873	0.040658739
3.4	0	0.019745022	0.024168466	0.038963423
3.5	0	0.019463886	0.022473508	0.037277682
3.6	0	0.019184347	0.020788005	0.035601398
3.7	0	0.018906415	0.019111841	0.033934454
3.8	0	0.018630099	0.017444901	0.032276735
3.9	0	0.018355409	0.015787074	0.030628129
4	0	0.01808235	0.014138251	0.028988528
4.1	0	0.017810929	0.012498323	0.027357823
4.2	0	0.01754115	0.010867187	0.025735911
4.3	0	0.017273019	0.009244739	0.024122688

4.4	0	0.017006537	0.007630879	0.022518054
4.5	0	0.016741708	0.00602551	0.020921911
4.6	0	0.016478533	0.004428533	0.019334162
4.7	0	0.016217012	0.002839856	0.017754712
4.8	0	0.015957147	0.001259384	0.016183469
4.9	0	0.015698938	-0.000312972	0.014620343
5	0	0.015442382	-0.001877301	0.013065243
5.1	0	0.01518748	-0.003433692	0.011518084
5.2	0	0.014934229	-0.004982229	0.009978778
5.3	0	0.014682628	-0.006522997	0.008447242
5.4	0	0.014432673	-0.008056078	0.006923395
5.5	0	0.014184362	-0.009581553	0.005407153
5.6	0	0.013937692	-0.011099501	0.003898439
5.7	0	0.013692658	-0.012610001	0.002397175
5.8	0	0.013449257	-0.014113128	0.000903283
5.9	0	0.013207485	-0.015608958	-0.000583311
6	0	0.012967337	-0.017097566	-0.002062682
6.1	0	0.012728808	-0.018579022	-0.003534901
6.2	0	0.012491894	-0.0200534	-0.005000041
6.3	0	0.01225659	-0.021520768	-0.00645817
6.4	0	0.01202289	-0.022981195	-0.007909359
6.5	0	0.011790789	-0.02443475	-0.009353674
6.6	0	0.01156028	-0.025881498	-0.010791182
6.7	0	0.011331359	-0.027321506	-0.012221949
6.8	0	0.01110402	-0.028754836	-0.013646039
6.9	0	0.010878256	-0.030181553	-0.015063514
7	0	0.010654061	-0.031601719	-0.016474438
7.1	0	0.010431428	-0.033015395	-0.017878871
7.2	0	0.010210353	-0.034422641	-0.019276874
7.3	0	0.009990828	-0.035823516	-0.020668506
7.4	0	0.009772846	-0.037218079	-0.022053825
7.5	0	0.009556401	-0.038606386	-0.023432888

7.6	0	0.009341487	-0.039988496	-0.024805753
7.7	0	0.009128096	-0.041364462	-0.026172474
7.8	0	0.008916222	-0.04273434	-0.027533106
7.9	0	0.008705858	-0.044098184	-0.028887704
8	0	0.008496998	-0.045456046	-0.03023632
8.1	0	0.008289634	-0.046807979	-0.031579007
8.2	0	0.008083759	-0.048154035	-0.032915816
8.3	0	0.007879367	-0.049494264	-0.034246798
8.4	0	0.007676451	-0.050828716	-0.035572003
8.5	0	0.007475003	-0.052157441	-0.03689148
8.6	0	0.007275017	-0.053480487	-0.038205277
8.7	0	0.007076486	-0.054797901	-0.039513443
8.8	0	0.006879402	-0.056109732	-0.040816025
8.9	0	0.006683759	-0.057416025	-0.042113069
9	0	0.00648955	-0.058716826	-0.043404621
9.1	0	0.006296768	-0.06001218	-0.044690725
9.2	0	0.006105405	-0.061302132	-0.045971428
9.3	0	0.005915455	-0.062586726	-0.047246772
9.4	0	0.005726911	-0.063866005	-0.048516801
9.5	0	0.005539766	-0.065140011	-0.049781557
9.6	0	0.005354013	-0.066408788	-0.051041083
9.7	0	0.005169645	-0.067672376	-0.052295421
9.8	0	0.004986655	-0.068930817	-0.05354461
9.9	0	0.004805036	-0.07018415	-0.054788692
10	0	0.004624782	-0.071432416	-0.056027707
10.1	0	0.004445885	-0.072675654	-0.057261694
10.2	0	0.00426834	-0.073913904	-0.058490692
10.3	0	0.004092138	-0.075147202	-0.059714739
10.4	0	0.003917273	-0.076375588	-0.060933874
10.5	0	0.003743739	-0.077599098	-0.062148132
10.6	0	0.00357153	-0.07881777	-0.063357552
10.7	0	0.003400636	-0.08003164	-0.06456217

10.8	0	0.003231054	-0.081240744	-0.065762022
10.9	0	0.003062776	-0.082445117	-0.066957143
11	0	0.002895794	-0.083644794	-0.068147568
11.1	0	0.002730104	-0.084839811	-0.069333332
11.2	0	0.002565698	-0.0860302	-0.07051447
11.3	0	0.00240257	-0.087215997	-0.071691014
11.4	0	0.002240713	-0.088397234	-0.072862999
11.5	0	0.002080121	-0.089573944	-0.074030457
11.6	0	0.001920788	-0.090746161	-0.075193422
11.7	0	0.001762707	-0.091913915	-0.076351923
11.8	0	0.001605872	-0.093077239	-0.077505995
11.9	0	0.001450276	-0.094236164	-0.078655668
12	0	0.001295914	-0.095390722	-0.079800974
12.1	0	0.00114278	-0.096540942	-0.080941942
12.2	0	0.000990866	-0.097686855	-0.082078604
12.3	0	0.000840167	-0.098828492	-0.083210988
12.4	0	0.000690677	-0.099965882	-0.084339126
12.5	0	0.000542391	-0.101099053	-0.085463046
12.6	0	0.0003953	-0.102228035	-0.086582776
12.7	0	0.000249401	-0.103352857	-0.087698347
12.8	0	0.000104687	-0.104473547	-0.088809785
12.9	0	-0.0000388485	-0.105590132	-0.089917119
13	0	-0.000181211	-0.106702641	-0.091020377
13.1	0	-0.000322405	-0.1078111	-0.092119585
13.2	0	-0.000462439	-0.108915538	-0.093214771
13.3	0	-0.000601316	-0.110015979	-0.094305962
13.4	0	-0.000739043	-0.111112452	-0.095393184
13.5	0	-0.000875626	-0.112204981	-0.096476464
13.6	0	-0.001011071	-0.113293594	-0.097555826
13.7	0	-0.001145381	-0.114378315	-0.098631297
13.8	0	-0.001278565	-0.115459169	-0.099702901
13.9	0	-0.001410626	-0.116536182	-0.100770665

14	0	-0.001541571	-0.117609379	-0.101834613
14.1	0	-0.001671404	-0.118678784	-0.102894769
14.2	0	-0.001800132	-0.119744422	-0.103951157
14.3	0	-0.00192776	-0.120806315	-0.105003802
14.4	0	-0.002054292	-0.121864489	-0.106052727
14.5	0	-0.002179735	-0.122918966	-0.107097956
14.6	0	-0.002304093	-0.123969769	-0.108139512
14.7	0	-0.002427373	-0.125016923	-0.109177417
14.8	0	-0.002549578	-0.126060449	-0.110211696
14.9	0	-0.002670714	-0.127100369	-0.11124237
15	0	-0.002790787	-0.128136708	-0.112269461
15.1	0	-0.002909801	-0.129169485	-0.113292992
15.2	0	-0.003027762	-0.130198724	-0.114312985
15.3	0	-0.003144674	-0.131224445	-0.115329461
15.4	0	-0.003260543	-0.132246671	-0.116342441
15.5	0	-0.003375373	-0.133265422	-0.117351947
15.6	0	-0.003489169	-0.13428072	-0.118358
15.7	0	-0.003601937	-0.135292585	-0.119360621
15.8	0	-0.003713681	-0.136301038	-0.120359829
15.9	0	-0.003824405	-0.137306099	-0.121355646
16	0	-0.003934116	-0.138307788	-0.122348092
16.1	0	-0.004042817	-0.139306125	-0.123337187
16.2	0	-0.004150513	-0.140301131	-0.12432295
16.3	0	-0.004257209	-0.141292825	-0.125305401
16.4	0	-0.00436291	-0.142281225	-0.12628456
16.5	0	-0.00446762	-0.143266352	-0.127260446
16.6	0	-0.004571344	-0.144248224	-0.128233077
16.7	0	-0.004674086	-0.145226861	-0.129202473
16.8	0	-0.004775851	-0.14620228	-0.130168652
16.9	0	-0.004876643	-0.147174501	-0.131131634
17	0	-0.004976467	-0.148143542	-0.132091435
17.1	0	-0.005075328	-0.14910942	-0.133048075

17.2	0	-0.005173229	-0.150072154	-0.134001571
17.3	0	-0.005270176	-0.151031763	-0.134951941
17.4	0	-0.005366171	-0.151988262	-0.135899203
17.5	0	-0.005461221	-0.152941671	-0.136843375
17.6	0	-0.005555328	-0.153892005	-0.137784474
17.7	0	-0.005648498	-0.154839283	-0.138722516
17.8	0	-0.005740735	-0.155783522	-0.139657519
17.9	0	-0.005832042	-0.156724738	-0.1405895
18	0	-0.005922424	-0.157662948	-0.141518476
18.1	0	-0.006011886	-0.158598168	-0.142444463
18.2	0	-0.00610043	-0.159530416	-0.143367477
18.3	0	-0.006188062	-0.160459707	-0.144287535
18.4	0	-0.006274785	-0.161386057	-0.145204654
18.5	0	-0.006360603	-0.162309483	-0.146118848
18.6	0	-0.006445521	-0.16323	-0.147030134
18.7	0	-0.006529542	-0.164147625	-0.147938528
18.8	0	-0.006612671	-0.165062371	-0.148844045
18.9	0	-0.006694911	-0.165974256	-0.1497467
19	0	-0.006776265	-0.166883295	-0.15064651
19.1	0	-0.006856739	-0.167789501	-0.151543488
19.2	0	-0.006936336	-0.168692892	-0.152437651
19.3	0	-0.00701506	-0.16959348	-0.153329013
19.4	0	-0.007092913	-0.170491282	-0.154217589
19.5	0	-0.007169902	-0.171386313	-0.155103393
19.6	0	-0.007246028	-0.172278585	-0.155986441
19.7	0	-0.007321296	-0.173168114	-0.156866745
19.8	0	-0.007395709	-0.174054915	-0.157744322
19.9	0	-0.007469272	-0.174939001	-0.158619185
20	0	-0.007541987	-0.175820387	-0.159491348

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2200 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.03140529	0.092476881	0.106813902
0.1	0	0.031094504	0.090364584	0.104710726
0.2	0	0.030781595	0.088267899	0.102623165
0.3	0	0.030466931	0.086186541	0.100550932
0.4	0	0.030150836	0.084120233	0.098493752
0.5	0	0.029833603	0.082068708	0.096451356
0.6	0	0.029515496	0.080031707	0.094423486
0.7	0	0.029196748	0.078008982	0.092409893
0.8	0	0.028877574	0.076000288	0.090410334
0.9	0	0.028558166	0.074005393	0.088424574
1	0	0.028238698	0.072024067	0.086452386
1.1	0	0.027919329	0.070056092	0.08449355
1.2	0	0.027600201	0.068101253	0.082547852
1.3	0	0.027281446	0.066159341	0.080615083
1.4	0	0.026963183	0.064230157	0.078695042
1.5	0	0.026645519	0.062313503	0.076787534
1.6	0	0.026328554	0.060409189	0.074892367
1.7	0	0.026012378	0.05851703	0.073009357
1.8	0	0.025697074	0.056636846	0.071138323
1.9	0	0.025382717	0.054768461	0.06927909
2	0	0.025069377	0.052911706	0.067431488
2.1	0	0.024757115	0.051066413	0.06559535
2.2	0	0.024445991	0.049232422	0.063770514
2.3	0	0.024136056	0.047409573	0.061956823
2.4	0	0.023827359	0.045597714	0.060154123
2.5	0	0.023519945	0.043796695	0.058362264
2.6	0	0.023213854	0.042006369	0.0565811

2.7	0	0.022909122	0.040226594	0.054810488
2.8	0	0.022605784	0.03845723	0.053050289
2.9	0	0.022303871	0.036698142	0.051300366
3	0	0.022003409	0.034949196	0.049560587
3.1	0	0.021704425	0.033210263	0.047830822
3.2	0	0.021406942	0.031481216	0.046110945
3.3	0	0.021110982	0.029761932	0.044400832
3.4	0	0.020816562	0.028052289	0.042700361
3.5	0	0.020523701	0.026352168	0.041009414
3.6	0	0.020232413	0.024661455	0.039327875
3.7	0	0.019942714	0.022980035	0.037655631
3.8	0	0.019654614	0.021307798	0.03599257
3.9	0	0.019368126	0.019644635	0.034338585
4	0	0.019083259	0.01799044	0.032693569
4.1	0	0.018800021	0.016345108	0.031057419
4.2	0	0.018518421	0.014708539	0.029430031
4.3	0	0.018238464	0.013080631	0.027811306
4.4	0	0.017960157	0.011461288	0.026201146
4.5	0	0.017683504	0.009850413	0.024599456
4.6	0	0.017408509	0.008247912	0.023006141
4.7	0	0.017135174	0.006653694	0.021421109
4.8	0	0.016863503	0.005067667	0.01984427
4.9	0	0.016593496	0.003489743	0.018275535
5	0	0.016325156	0.001919835	0.016714817
5.1	0	0.016058482	0.000357858	0.015162031
5.2	0	0.015793475	-0.001196271	0.013617093
5.3	0	0.015530133	-0.002742636	0.012079921
5.4	0	0.015268457	-0.004281317	0.010550434
5.5	0	0.015008444	-0.005812393	0.009028553
5.6	0	0.014750092	-0.007335941	0.0075142
5.7	0	0.0144934	-0.008852039	0.006007299
5.8	0	0.014238364	-0.010360761	0.004507774

5.9	0	0.013984982	-0.011862181	0.003015553
6	0	0.013733251	-0.013356371	0.001530562
6.1	0	0.013483167	-0.014843402	0.0000527298
6.2	0	0.013234725	-0.016323346	-0.001418013
6.3	0	0.012987923	-0.017796269	-0.002881735
6.4	0	0.012742756	-0.019262241	-0.004338504
6.5	0	0.012499219	-0.020721327	-0.005788387
6.6	0	0.012257308	-0.022173592	-0.007231448
6.7	0	0.012017017	-0.023619102	-0.008667754
6.8	0	0.011778342	-0.02505792	-0.010097366
6.9	0	0.011541278	-0.026490106	-0.011520346
7	0	0.011305819	-0.027915724	-0.012936757
7.1	0	0.011071959	-0.029334833	-0.014346659
7.2	0	0.010839694	-0.030747493	-0.01575011
7.3	0	0.010609017	-0.032153761	-0.01714717
7.4	0	0.010379922	-0.033553696	-0.018537895
7.5	0	0.010152403	-0.034947353	-0.019922342
7.6	0	0.009926456	-0.03633479	-0.021300568
7.7	0	0.009702072	-0.03771606	-0.022672626
7.8	0	0.009479247	-0.039091217	-0.024038572
7.9	0	0.009257973	-0.040460315	-0.025398457
8	0	0.009038245	-0.041823407	-0.026752335
8.1	0	0.008820057	-0.043180543	-0.028100258
8.2	0	0.008603401	-0.044531775	-0.029442275
8.3	0	0.008388271	-0.045877153	-0.030778439
8.4	0	0.008174662	-0.047216727	-0.032108797
8.5	0	0.007962565	-0.048550544	-0.033433398
8.6	0	0.007751975	-0.049878654	-0.034752291
8.7	0	0.007542885	-0.051201103	-0.036065523
8.8	0	0.007335289	-0.052517938	-0.03737314
8.9	0	0.00712918	-0.053829205	-0.03867519
9	0	0.00692455	-0.055134949	-0.039971716

9.1	0	0.006721395	-0.056435216	-0.041262764
9.2	0	0.006519706	-0.057730049	-0.042548378
9.3	0	0.006319477	-0.059019492	-0.043828601
9.4	0	0.006120701	-0.060303588	-0.045103476
9.5	0	0.005923373	-0.061582379	-0.046373047
9.6	0	0.005727484	-0.062855906	-0.047637354
9.7	0	0.005533029	-0.064124212	-0.048896438
9.8	0	0.005340001	-0.065387337	-0.050150341
9.9	0	0.005148392	-0.06664532	-0.051399102
10	0	0.004958198	-0.067898203	-0.052642762
10.1	0	0.004769409	-0.069146023	-0.05388136
10.2	0	0.004582021	-0.070388819	-0.055114933
10.3	0	0.004396027	-0.071626629	-0.05634352
10.4	0	0.004211419	-0.072859491	-0.057567158
10.5	0	0.004028192	-0.074087443	-0.058785886
10.6	0	0.003846339	-0.07531052	-0.059999739
10.7	0	0.003665853	-0.07652876	-0.061208754
10.8	0	0.003486727	-0.077742197	-0.062412966
10.9	0	0.003308956	-0.078950867	-0.063612412
11	0	0.003132533	-0.080154805	-0.064807124
11.1	0	0.002957451	-0.081354045	-0.065997139
11.2	0	0.002783704	-0.082548622	-0.067182491
11.3	0	0.002611285	-0.083738569	-0.068363212
11.4	0	0.002440189	-0.084923919	-0.069539336
11.5	0	0.002270408	-0.086104705	-0.070710896
11.6	0	0.002101937	-0.08728096	-0.071877924
11.7	0	0.001934769	-0.088452715	-0.073040453
11.8	0	0.001768898	-0.089620002	-0.074198513
11.9	0	0.001604318	-0.090782853	-0.075352137
12	0	0.001441023	-0.091941298	-0.076501355
12.1	0	0.001279006	-0.093095368	-0.077646198
12.2	0	0.001118261	-0.094245093	-0.078786696

12.3	0	0.000958782	-0.095390503	-0.079922878
12.4	0	0.000800564	-0.096531627	-0.081054776
12.5	0	0.000643599	-0.097668495	-0.082182416
12.6	0	0.000487883	-0.098801136	-0.083305829
12.7	0	0.000333408	-0.099929577	-0.084425044
12.8	0	0.00018017	-0.101053848	-0.085540087
12.9	0	0.0000281626	-0.102173976	-0.086650987
13	0	-0.000122621	-0.103289989	-0.087757773
13.1	0	-0.000272186	-0.104401914	-0.08886047
13.2	0	-0.000420538	-0.105509778	-0.089959106
13.3	0	-0.000567683	-0.106613607	-0.091053708
13.4	0	-0.000713626	-0.107713429	-0.092144302
13.5	0	-0.000858375	-0.108809268	-0.093230914
13.6	0	-0.001001933	-0.109901152	-0.09431357
13.7	0	-0.001144307	-0.110989105	-0.095392296
13.8	0	-0.001285502	-0.112073153	-0.096467116
13.9	0	-0.001425525	-0.113153321	-0.097538057
14	0	-0.001564379	-0.114229634	-0.098605142
14.1	0	-0.001702072	-0.115302115	-0.099668397
14.2	0	-0.001838607	-0.11637079	-0.100727844
14.3	0	-0.001973992	-0.117435682	-0.101783509
14.4	0	-0.002108231	-0.118496816	-0.102835416
14.5	0	-0.002241329	-0.119554213	-0.103883586
14.6	0	-0.002373293	-0.120607898	-0.104928045
14.7	0	-0.002504126	-0.121657895	-0.105968815
14.8	0	-0.002633835	-0.122704224	-0.107005918
14.9	0	-0.002762425	-0.12374691	-0.108039377
15	0	-0.0028899	-0.124785974	-0.109069215
15.1	0	-0.003016267	-0.125821438	-0.110095454
15.2	0	-0.00314153	-0.126853325	-0.111118115
15.3	0	-0.003265694	-0.127881656	-0.11213722
15.4	0	-0.003388764	-0.128906452	-0.113152791

15.5	0	-0.003510745	-0.129927735	-0.114164848
15.6	0	-0.003631643	-0.130945525	-0.115173414
15.7	0	-0.003751463	-0.131959844	-0.116178508
15.8	0	-0.003870208	-0.132970712	-0.117180151
15.9	0	-0.003987885	-0.133978149	-0.118178365
16	0	-0.004104497	-0.134982176	-0.119173168
16.1	0	-0.004220051	-0.135982813	-0.120164581
16.2	0	-0.00433455	-0.136980079	-0.121152624
16.3	0	-0.004447999	-0.137973994	-0.122137316
16.4	0	-0.004560404	-0.138964578	-0.123118677
16.5	0	-0.004671769	-0.13995185	-0.124096726
16.6	0	-0.004782098	-0.140935829	-0.125071483
16.7	0	-0.004891397	-0.141916534	-0.126042965
16.8	0	-0.004999669	-0.142893983	-0.127011193
16.9	0	-0.00510692	-0.143868195	-0.127976184
17	0	-0.005213154	-0.144839189	-0.128937957
17.1	0	-0.005318375	-0.145806983	-0.12989653
17.2	0	-0.005422589	-0.146771594	-0.130851921
17.3	0	-0.005525799	-0.147733041	-0.131804149
17.4	0	-0.00562801	-0.148691342	-0.132753229
17.5	0	-0.005729226	-0.149646513	-0.133699182
17.6	0	-0.005829452	-0.150598573	-0.134642023
17.7	0	-0.005928692	-0.151547538	-0.13558177
17.8	0	-0.006026951	-0.152493426	-0.13651844
17.9	0	-0.006124233	-0.153436254	-0.13745205
18	0	-0.006220541	-0.154376038	-0.138382616
18.1	0	-0.006315881	-0.155312795	-0.139310157
18.2	0	-0.006410257	-0.156246542	-0.140234687
18.3	0	-0.006503672	-0.157177294	-0.141156223
18.4	0	-0.00659613	-0.158105068	-0.142074782
18.5	0	-0.006687637	-0.159029881	-0.14299038
18.6	0	-0.006778196	-0.159951747	-0.143903032

18.7	0	-0.006867812	-0.160870684	-0.144812754
18.8	0	-0.006956487	-0.161786705	-0.145719562
18.9	0	-0.007044227	-0.162699828	-0.146623472
19	0	-0.007131035	-0.163610067	-0.147524498
19.1	0	-0.007216915	-0.164517438	-0.148422657
19.2	0	-0.007301872	-0.165421955	-0.149317963
19.3	0	-0.007385908	-0.166323634	-0.150210431
19.4	0	-0.007469029	-0.16722249	-0.151100075
19.5	0	-0.007551238	-0.168118537	-0.151986912
19.6	0	-0.007632538	-0.16901179	-0.152870956
19.7	0	-0.007712934	-0.169902263	-0.15375222
19.8	0	-0.007792429	-0.170789971	-0.154630719
19.9	0	-0.007871028	-0.171674928	-0.155506468
20	0	-0.007948734	-0.172557148	-0.156379481

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2300 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.032839881	0.096405841	0.110595609
0.1	0	0.032522389	0.094294707	0.108493553
0.2	0	0.032202464	0.09219882	0.106406746
0.3	0	0.031880489	0.090117912	0.10433492
0.4	0	0.031556806	0.088051725	0.102277817
0.5	0	0.031231722	0.086000009	0.100235188
0.6	0	0.030905513	0.083962521	0.098206788
0.7	0	0.03057843	0.081939028	0.096192385
0.8	0	0.030250698	0.079929299	0.094191749
0.9	0	0.029922521	0.077933116	0.092204659
1	0	0.029594086	0.075950263	0.090230902
1.1	0	0.029265561	0.073980531	0.088270268

1.2	0	0.028937102	0.072023719	0.086322556
1.3	0	0.028608847	0.07007963	0.084387568
1.4	0	0.028280926	0.068148072	0.082465113
1.5	0	0.027953455	0.06622886	0.080555006
1.6	0	0.027626543	0.064321812	0.078657065
1.7	0	0.027300288	0.062426752	0.076771114
1.8	0	0.02697478	0.060543509	0.074896981
1.9	0	0.026650103	0.058671915	0.073034499
2	0	0.026326331	0.056811808	0.071183506
2.1	0	0.026003535	0.054963028	0.069343842
2.2	0	0.02568178	0.053125422	0.067515352
2.3	0	0.025361123	0.051298837	0.065697887
2.4	0	0.02504162	0.049483127	0.063891297
2.5	0	0.02472332	0.047678149	0.06209544
2.6	0	0.024406269	0.04588376	0.060310175
2.7	0	0.024090508	0.044099825	0.058535365
2.8	0	0.023776077	0.042326209	0.056770876
2.9	0	0.023463012	0.040562782	0.055016578
3	0	0.023151343	0.038809415	0.053272341
3.1	0	0.022841102	0.037065984	0.051538042
3.2	0	0.022532315	0.035332367	0.049813557
3.3	0	0.022225008	0.033608443	0.048098768
3.4	0	0.021919203	0.031894097	0.046393557
3.5	0	0.021614921	0.030189212	0.04469781
3.6	0	0.021312181	0.028493678	0.043011414
3.7	0	0.021011001	0.026807384	0.041334261
3.8	0	0.020711395	0.025130224	0.039666242
3.9	0	0.020413379	0.023462092	0.038007252
4	0	0.020116964	0.021802885	0.036357189
4.1	0	0.019822162	0.020152501	0.034715952
4.2	0	0.019528984	0.018510843	0.03308344
4.3	0	0.019237438	0.016877812	0.031459558

4.4	0	0.018947533	0.015253314	0.029844209
4.5	0	0.018659275	0.013637256	0.028237302
4.6	0	0.018372671	0.012029546	0.026638744
4.7	0	0.018087726	0.010430095	0.025048446
4.8	0	0.017804445	0.008838813	0.023466319
4.9	0	0.01752283	0.007255616	0.021892277
5	0	0.017242886	0.005680418	0.020326236
5.1	0	0.016964614	0.004113135	0.018768112
5.2	0	0.016688016	0.002553687	0.017217823
5.3	0	0.016413094	0.001001993	0.015675289
5.4	0	0.016139847	-0.000542027	0.014140431
5.5	0	0.015868277	-0.002078448	0.012613172
5.6	0	0.015598383	-0.003607348	0.011093436
5.7	0	0.015330164	-0.005128801	0.009581148
5.8	0	0.015063619	-0.006642881	0.008076234
5.9	0	0.014798746	-0.008149659	0.006578623
6	0	0.014535543	-0.009649208	0.005088242
6.1	0	0.014274009	-0.011141595	0.003605024
6.2	0	0.01401414	-0.012626891	0.002128898
6.3	0	0.013755933	-0.014105163	0.000659798
6.4	0	0.013499386	-0.015576476	-0.000802343
6.5	0	0.013244495	-0.017040896	-0.00225759
6.6	0	0.012991257	-0.018498488	-0.003706008
6.7	0	0.012739667	-0.019949314	-0.005147659
6.8	0	0.012489721	-0.021393437	-0.006582607
6.9	0	0.012241416	-0.022830918	-0.00801091
7	0	0.011994746	-0.024261817	-0.009432632
7.1	0	0.011749707	-0.025686193	-0.010847829
7.2	0	0.011506294	-0.027104106	-0.012256562
7.3	0	0.011264503	-0.028515611	-0.013658887
7.4	0	0.011024328	-0.029920766	-0.015054861
7.5	0	0.010785764	-0.031319627	-0.01644454

7.6	0	0.010548805	-0.032712248	-0.017827978
7.7	0	0.010313447	-0.034098683	-0.01920523
7.8	0	0.010079683	-0.035478987	-0.020576348
7.9	0	0.009847509	-0.03685321	-0.021941387
8	0	0.009616918	-0.038221406	-0.023300396
8.1	0	0.009387904	-0.039583624	-0.024653428
8.2	0	0.009160462	-0.040939916	-0.026000532
8.3	0	0.008934586	-0.04229033	-0.027341758
8.4	0	0.008710269	-0.043634916	-0.028677155
8.5	0	0.008487506	-0.044973721	-0.030006771
8.6	0	0.00826629	-0.046306794	-0.031330653
8.7	0	0.008046616	-0.04763418	-0.032648848
8.8	0	0.007828478	-0.048955926	-0.033961403
8.9	0	0.007611868	-0.050272078	-0.035268362
9	0	0.007396781	-0.05158268	-0.036569771
9.1	0	0.007183211	-0.052887777	-0.037865674
9.2	0	0.006971151	-0.054187411	-0.039156115
9.3	0	0.006760594	-0.055481627	-0.040441136
9.4	0	0.006551535	-0.056770467	-0.04172078
9.5	0	0.006343968	-0.058053973	-0.04299509
9.6	0	0.006137885	-0.059332186	-0.044264106
9.7	0	0.00593328	-0.060605146	-0.04552787
9.8	0	0.005730148	-0.061872895	-0.046786422
9.9	0	0.005528481	-0.063135472	-0.0480398
10	0	0.005328273	-0.064392917	-0.049288046
10.1	0	0.005129518	-0.065645267	-0.050531198
10.2	0	0.00493221	-0.066892562	-0.051769293
10.3	0	0.004736341	-0.068134839	-0.05300237
10.4	0	0.004541907	-0.069372136	-0.054230466
10.5	0	0.004348899	-0.070604489	-0.055453618
10.6	0	0.004157313	-0.071831935	-0.056671862
10.7	0	0.003967141	-0.073054509	-0.057885235

10.8	0	0.003778377	-0.074272248	-0.059093771
10.9	0	0.003591015	-0.075485186	-0.060297507
11	0	0.003405049	-0.076693358	-0.061496475
11.1	0	0.003220472	-0.077896798	-0.062690712
11.2	0	0.003037278	-0.07909554	-0.06388025
11.3	0	0.00285546	-0.080289617	-0.065065124
11.4	0	0.002675014	-0.081479063	-0.066245365
11.5	0	0.002495931	-0.08266391	-0.067421007
11.6	0	0.002318207	-0.08384419	-0.068592082
11.7	0	0.002141835	-0.085019936	-0.069758621
11.8	0	0.001966808	-0.086191177	-0.070920658
11.9	0	0.001793121	-0.087357947	-0.072078221
12	0	0.001620768	-0.088520275	-0.073231343
12.1	0	0.001449742	-0.089678192	-0.074380053
12.2	0	0.001280037	-0.090831728	-0.075524382
12.3	0	0.001111648	-0.091980913	-0.07666436
12.4	0	0.000944568	-0.093125776	-0.077800015
12.5	0	0.000778791	-0.094266346	-0.078931378
12.6	0	0.000614312	-0.095402652	-0.080058476
12.7	0	0.000451125	-0.096534723	-0.081181338
12.8	0	0.000289223	-0.097662586	-0.082299993
12.9	0	0.000128601	-0.098786269	-0.083414468
13	0	-0.0000307474	-0.0999058	-0.08452479
13.1	0	-0.000188828	-0.101021206	-0.085630987
13.2	0	-0.000345645	-0.102132513	-0.086733086
13.3	0	-0.000501207	-0.10323975	-0.087831113
13.4	0	-0.000655517	-0.10434294	-0.088925095
13.5	0	-0.000808582	-0.105442112	-0.090015057
13.6	0	-0.000960408	-0.106537291	-0.091101026
13.7	0	-0.001110999	-0.107628501	-0.092183027
13.8	0	-0.001260363	-0.108715769	-0.093261085
13.9	0	-0.001408504	-0.109799119	-0.094335226

14	0	-0.001555427	-0.110878576	-0.095405473
14.1	0	-0.001701139	-0.111954165	-0.096471851
14.2	0	-0.001845645	-0.113025909	-0.097534385
14.3	0	-0.00198895	-0.114093832	-0.098593099
14.4	0	-0.002131059	-0.115157959	-0.099648016
14.5	0	-0.002271979	-0.116218313	-0.10069916
14.6	0	-0.002411714	-0.117274917	-0.101746553
14.7	0	-0.00255027	-0.118327793	-0.10279022
14.8	0	-0.002687652	-0.119376965	-0.103830182
14.9	0	-0.002823865	-0.120422456	-0.104866462
15	0	-0.002958914	-0.121464287	-0.105899083
15.1	0	-0.003092805	-0.12250248	-0.106928066
15.2	0	-0.003225544	-0.123537058	-0.107953434
15.3	0	-0.003357134	-0.124568042	-0.108975208
15.4	0	-0.003487581	-0.125595454	-0.10999341
15.5	0	-0.003616891	-0.126619314	-0.111008061
15.6	0	-0.003745067	-0.127639644	-0.112019181
15.7	0	-0.003872116	-0.128656465	-0.113026792
15.8	0	-0.003998042	-0.129669796	-0.114030914
15.9	0	-0.004122851	-0.13067966	-0.115031568
16	0	-0.004246546	-0.131686075	-0.116028774
16.1	0	-0.004369134	-0.132689062	-0.117022552
16.2	0	-0.004490618	-0.133688641	-0.118012922
16.3	0	-0.004611005	-0.134684832	-0.118999903
16.4	0	-0.004730297	-0.135677653	-0.119983516
16.5	0	-0.004848501	-0.136667124	-0.120963778
16.6	0	-0.004965622	-0.137653264	-0.12194071
16.7	0	-0.005081663	-0.138636093	-0.122914331
16.8	0	-0.005196629	-0.139615629	-0.123884658
16.9	0	-0.005310526	-0.14059189	-0.124851711
17	0	-0.005423357	-0.141564895	-0.125815509
17.1	0	-0.005535128	-0.142534662	-0.126776068

17.2	0	-0.005645842	-0.143501209	-0.127733408
17.3	0	-0.005755506	-0.144464555	-0.128687547
17.4	0	-0.005864122	-0.145424716	-0.129638502
17.5	0	-0.005971696	-0.146381711	-0.13058629
17.6	0	-0.006078231	-0.147335557	-0.13153093
17.7	0	-0.006183734	-0.148286272	-0.132472438
17.8	0	-0.006288206	-0.149233871	-0.133410832
17.9	0	-0.006391655	-0.150178373	-0.134346128
18	0	-0.006494083	-0.151119794	-0.135278344
18.1	0	-0.006595494	-0.152058151	-0.136207496
18.2	0	-0.006695894	-0.152993461	-0.137133601
18.3	0	-0.006795287	-0.153925739	-0.138056675
18.4	0	-0.006893676	-0.154855002	-0.138976734
18.5	0	-0.006991066	-0.155781266	-0.139893795
18.6	0	-0.007087461	-0.156704548	-0.140807873
18.7	0	-0.007182865	-0.157624862	-0.141718984
18.8	0	-0.007277283	-0.158542225	-0.142627144
18.9	0	-0.007370719	-0.159456652	-0.143532369
19	0	-0.007463176	-0.160368159	-0.144434674
19.1	0	-0.007554659	-0.161276761	-0.145334074
19.2	0	-0.007645172	-0.162182472	-0.146230585
19.3	0	-0.007734718	-0.163085309	-0.147124221
19.4	0	-0.007823303	-0.163985286	-0.148014998
19.5	0	-0.007910929	-0.164882418	-0.148902929
19.6	0	-0.007997601	-0.16577672	-0.149788031
19.7	0	-0.008083322	-0.166668205	-0.150670317
19.8	0	-0.008168097	-0.167556889	-0.151549803
19.9	0	-0.008251929	-0.168442786	-0.152426501
20	0	-0.008334823	-0.16932591	-0.153300427

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2400 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.034275919	0.100281001	0.114329288
0.1	0	0.033952006	0.098171496	0.112228839
0.2	0	0.033625359	0.096076876	0.110143277
0.3	0	0.033296376	0.093996892	0.108072353
0.4	0	0.032965412	0.091931302	0.106015824
0.5	0	0.03263279	0.089879871	0.103973458
0.6	0	0.032298798	0.087842373	0.101945026
0.7	0	0.031963699	0.085818588	0.099930308
0.8	0	0.031627731	0.083808299	0.097929089
0.9	0	0.031291109	0.081811301	0.095941163
1	0	0.03095403	0.079827389	0.093966325
1.1	0	0.030616673	0.077856368	0.092004379
1.2	0	0.030279203	0.075898046	0.090055135
1.3	0	0.029941769	0.073952238	0.088118406
1.4	0	0.029604509	0.072018761	0.08619401
1.5	0	0.029267549	0.07009744	0.084281771
1.6	0	0.028931004	0.068188102	0.082381518
1.7	0	0.02859498	0.06629058	0.080493082
1.8	0	0.028259575	0.06440471	0.078616301
1.9	0	0.02792488	0.062530334	0.076751015
2	0	0.027590977	0.060667296	0.074897068
2.1	0	0.027257943	0.058815445	0.07305431
2.2	0	0.026925847	0.056974632	0.071222592
2.3	0	0.026594755	0.055144713	0.06940177
2.4	0	0.026264727	0.053325548	0.067591702
2.5	0	0.025935817	0.051516998	0.065792252
2.6	0	0.025608078	0.049718928	0.064003284

2.7	0	0.025281555	0.047931208	0.062224667
2.8	0	0.024956293	0.046153709	0.060456273
2.9	0	0.024632332	0.044386305	0.058697974
3	0	0.024309707	0.042628872	0.056949649
3.1	0	0.023988454	0.040881292	0.055211178
3.2	0	0.023668604	0.039143445	0.053482441
3.3	0	0.023350186	0.037415216	0.051763325
3.4	0	0.023033226	0.035696493	0.050053716
3.5	0	0.022717748	0.033987166	0.048353503
3.6	0	0.022403775	0.032287125	0.046662579
3.7	0	0.022091328	0.030596265	0.044980837
3.8	0	0.021780425	0.028914482	0.043308173
3.9	0	0.021471083	0.027241675	0.041644486
4	0	0.021163319	0.025577743	0.039989676
4.1	0	0.020857146	0.023922588	0.038343645
4.2	0	0.020552577	0.022276116	0.036706297
4.3	0	0.020249625	0.02063823	0.035077537
4.4	0	0.019948299	0.01900884	0.033457274
4.5	0	0.019648608	0.017387855	0.031845417
4.6	0	0.019350563	0.015775185	0.030241877
4.7	0	0.019054169	0.014170744	0.028646567
4.8	0	0.018759434	0.012574446	0.0270594
4.9	0	0.018466364	0.010986206	0.025480294
5	0	0.018174963	0.009405943	0.023909165
5.1	0	0.017885235	0.007833575	0.022345933
5.2	0	0.017597185	0.006269022	0.020790517
5.3	0	0.017310815	0.004712206	0.01924284
5.4	0	0.017026128	0.003163051	0.017702824
5.5	0	0.016743125	0.001621481	0.016170394
5.6	0	0.016461808	0.0000874212	0.014645476
5.7	0	0.016182177	-0.001439201	0.013127996
5.8	0	0.015904233	-0.002958458	0.011617883

5.9	0	0.015627975	-0.004470419	0.010115066
6	0	0.015353403	-0.005975154	0.008619476
6.1	0	0.015080516	-0.007472732	0.007131045
6.2	0	0.014809314	-0.00896322	0.005649705
6.3	0	0.014539793	-0.010446683	0.00417539
6.4	0	0.014271952	-0.011923187	0.002708036
6.5	0	0.014005789	-0.013392796	0.001247578
6.6	0	0.013741301	-0.014855572	-0.000206047
6.7	0	0.013478486	-0.016311578	-0.0016529
6.8	0	0.01321734	-0.017760874	-0.003093042
6.9	0	0.01295786	-0.019203521	-0.004526535
7	0	0.012700043	-0.020639577	-0.005953436
7.1	0	0.012443885	-0.022069101	-0.007373804
7.2	0	0.012189381	-0.023492151	-0.008787697
7.3	0	0.011936529	-0.024908782	-0.01019517
7.4	0	0.011685323	-0.026319051	-0.01159628
7.5	0	0.011435759	-0.027723011	-0.012991081
7.6	0	0.011187833	-0.029120718	-0.014379628
7.7	0	0.010941539	-0.030512224	-0.015761973
7.8	0	0.010696874	-0.031897582	-0.017138169
7.9	0	0.010453832	-0.033276844	-0.018508267
8	0	0.010212408	-0.034650059	-0.01987232
8.1	0	0.009972597	-0.03601728	-0.021230376
8.2	0	0.009734393	-0.037378554	-0.022582485
8.3	0	0.009497792	-0.038733931	-0.023928697
8.4	0	0.009262788	-0.04008346	-0.025269059
8.5	0	0.009029375	-0.041427187	-0.026603619
8.6	0	0.008797548	-0.042765159	-0.027932423
8.7	0	0.008567301	-0.044097422	-0.029255518
8.8	0	0.008338628	-0.045424023	-0.030572949
8.9	0	0.008111524	-0.046745005	-0.031884762
9	0	0.007885984	-0.048060414	-0.033191

9.1	0	0.007662	-0.049370292	-0.034491708
9.2	0	0.007439567	-0.050674684	-0.035786928
9.3	0	0.00721868	-0.051973631	-0.037076703
9.4	0	0.006999332	-0.053267176	-0.038361075
9.5	0	0.006781517	-0.05455536	-0.039640086
9.6	0	0.00656523	-0.055838224	-0.040913776
9.7	0	0.006350464	-0.057115808	-0.042182186
9.8	0	0.006137213	-0.058388153	-0.043445356
9.9	0	0.005925471	-0.059655298	-0.044703325
10	0	0.005715232	-0.060917281	-0.045956133
10.1	0	0.005506491	-0.062174141	-0.047203817
10.2	0	0.00529924	-0.063425916	-0.048446415
10.3	0	0.005093473	-0.064672644	-0.049683965
10.4	0	0.004889186	-0.065914361	-0.050916504
10.5	0	0.00468637	-0.067151104	-0.052144068
10.6	0	0.004485022	-0.068382908	-0.053366694
10.7	0	0.004285133	-0.06960981	-0.054584417
10.8	0	0.004086699	-0.070831845	-0.055797273
10.9	0	0.003889712	-0.072049048	-0.057005295
11	0	0.003694167	-0.073261452	-0.058208519
11.1	0	0.003500059	-0.074469092	-0.059406979
11.2	0	0.003307379	-0.075672002	-0.060600708
11.3	0	0.003116123	-0.076870215	-0.061789739
11.4	0	0.002926285	-0.078063763	-0.062974105
11.5	0	0.002737859	-0.079252678	-0.064153838
11.6	0	0.002550837	-0.080436994	-0.065328971
11.7	0	0.002365215	-0.081616741	-0.066499536
11.8	0	0.002180986	-0.08279195	-0.067665562
11.9	0	0.001998145	-0.083962654	-0.068827082
12	0	0.001816685	-0.085128881	-0.069984126
12.1	0	0.0016366	-0.086290663	-0.071136725
12.2	0	0.001457885	-0.08744803	-0.072284907

12.3	0	0.001280533	-0.08860101	-0.073428703
12.4	0	0.001104539	-0.089749634	-0.074568142
12.5	0	0.000929896	-0.09089393	-0.075703253
12.6	0	0.000756599	-0.092033926	-0.076834065
12.7	0	0.000584643	-0.093169652	-0.077960605
12.8	0	0.00041402	-0.094301134	-0.079082902
12.9	0	0.000244726	-0.095428401	-0.080200984
13	0	0.0000767543	-0.09655148	-0.081314877
13.1	0	-0.0000899006	-0.097670399	-0.082424609
13.2	0	-0.000255244	-0.098785183	-0.083530207
13.3	0	-0.000419283	-0.099895859	-0.084631697
13.4	0	-0.000582021	-0.101002454	-0.085729106
13.5	0	-0.000743466	-0.102104993	-0.086822459
13.6	0	-0.000903622	-0.103203503	-0.087911782
13.7	0	-0.001062495	-0.104298008	-0.088997101
13.8	0	-0.001220091	-0.105388535	-0.09007844
13.9	0	-0.001376415	-0.106475106	-0.091155825
14	0	-0.001531473	-0.107557748	-0.09222928
14.1	0	-0.00168527	-0.108636485	-0.09329883
14.2	0	-0.001837812	-0.10971134	-0.094364499
14.3	0	-0.001989104	-0.110782339	-0.09542631
14.4	0	-0.002139152	-0.111849503	-0.096484287
14.5	0	-0.002287961	-0.112912857	-0.097538454
14.6	0	-0.002435536	-0.113972424	-0.098588834
14.7	0	-0.002581882	-0.115028227	-0.09963545
14.8	0	-0.002727006	-0.116080288	-0.100678324
14.9	0	-0.002870912	-0.11712863	-0.101717479
15	0	-0.003013605	-0.118173276	-0.102752938
15.1	0	-0.003155091	-0.119214247	-0.103784722
15.2	0	-0.003295375	-0.120251564	-0.104812853
15.3	0	-0.003434462	-0.121285251	-0.105837352
15.4	0	-0.003572357	-0.122315328	-0.106858242

15.5	0	-0.003709065	-0.123341816	-0.107875544
15.6	0	-0.003844592	-0.124364737	-0.108889278
15.7	0	-0.003978942	-0.125384111	-0.109899465
15.8	0	-0.00411212	-0.126399958	-0.110906126
15.9	0	-0.004244132	-0.1274123	-0.111909282
16	0	-0.004374982	-0.128421156	-0.112908952
16.1	0	-0.004504676	-0.129426546	-0.113905156
16.2	0	-0.004633217	-0.130428491	-0.114897915
16.3	0	-0.004760612	-0.13142701	-0.115887248
16.4	0	-0.004886865	-0.132422122	-0.116873174
16.5	0	-0.00501198	-0.133413847	-0.117855713
16.6	0	-0.005135963	-0.134402203	-0.118834884
16.7	0	-0.005258818	-0.13538721	-0.119810706
16.8	0	-0.005380551	-0.136368887	-0.120783198
16.9	0	-0.005501165	-0.137347251	-0.121752378
17	0	-0.005620665	-0.138322323	-0.122718265
17.1	0	-0.005739057	-0.139294119	-0.123680876
17.2	0	-0.005856345	-0.140262657	-0.124640231
17.3	0	-0.005972532	-0.141227957	-0.125596347
17.4	0	-0.006087625	-0.142190035	-0.126549241
17.5	0	-0.006201628	-0.143148909	-0.127498932
17.6	0	-0.006314544	-0.144104597	-0.128445437
17.7	0	-0.006426379	-0.145057116	-0.129388773
17.8	0	-0.006537137	-0.146006483	-0.130328957
17.9	0	-0.006646822	-0.146952715	-0.131266007
18	0	-0.006755439	-0.147895829	-0.132199939
18.1	0	-0.006862993	-0.148835841	-0.133130769
18.2	0	-0.006969487	-0.149772769	-0.134058516
18.3	0	-0.007074926	-0.150706629	-0.134983194
18.4	0	-0.007179314	-0.151637436	-0.135904821
18.5	0	-0.007282656	-0.152565207	-0.136823412
18.6	0	-0.007384956	-0.153489959	-0.137738983

18.7	0	-0.007486218	-0.154411706	-0.138651551
18.8	0	-0.007586446	-0.155330465	-0.139561131
18.9	0	-0.007685645	-0.156246252	-0.140467738
19	0	-0.007783819	-0.157159081	-0.141371388
19.1	0	-0.007880971	-0.158068968	-0.142272097
19.2	0	-0.007977106	-0.158975928	-0.14316988
19.3	0	-0.008072229	-0.159879977	-0.144064751
19.4	0	-0.008166342	-0.160781129	-0.144956726
19.5	0	-0.008259451	-0.1616794	-0.14584582
19.6	0	-0.008351558	-0.162574803	-0.146732047
19.7	0	-0.008442669	-0.163467354	-0.147615422
19.8	0	-0.008532787	-0.164357066	-0.148495959
19.9	0	-0.008621917	-0.165243955	-0.149373673
20	0	-0.008710061	-0.166128035	-0.150248578

The Gibbs free energy difference of the four polytypes of boron nitride (r-BN, h-BN, c-BN, and w-BN) as a function of pressure ranging from 0 to 20 GPa, calculated with respect to r-BN as a reference at **a given temperature of 2500 Kelvin**. The unit of the Gibbs free energy difference for the four polytypes of boron nitride is given in eV/atom.

P(GPa)	r-BN	h-BN	c-BN	w-BN
0	0	0.035716515	0.104093232	0.117995713
0.1	0	0.035386504	0.101985889	0.115897379
0.2	0	0.035053466	0.099893076	0.113813577
0.3	0	0.034717813	0.097814562	0.111744076
0.4	0	0.034379916	0.095750121	0.10968865
0.5	0	0.034040107	0.093699532	0.107647078
0.6	0	0.033698688	0.091662583	0.105619148
0.7	0	0.033355932	0.089639067	0.103604653
0.8	0	0.033012089	0.087628781	0.10160339
0.9	0	0.032667385	0.085631531	0.099615164
1	0	0.032322027	0.083647125	0.097639785
1.1	0	0.031976203	0.081675377	0.095677066

1.2	0	0.031630088	0.079716107	0.093726826
1.3	0	0.031283838	0.077769139	0.09178889
1.4	0	0.030937601	0.0758343	0.089863085
1.5	0	0.03059151	0.073911424	0.087949244
1.6	0	0.030245689	0.072000346	0.086047205
1.7	0	0.029900252	0.070100909	0.084156807
1.8	0	0.029555302	0.068212957	0.082277896
1.9	0	0.029210938	0.066336337	0.080410319
2	0	0.028867248	0.064470903	0.078553929
2.1	0	0.028524315	0.062616509	0.076708582
2.2	0	0.028182215	0.060773014	0.074874135
2.3	0	0.027841019	0.058940281	0.073050451
2.4	0	0.027500793	0.057118174	0.071237395
2.5	0	0.027161596	0.055306561	0.069434835
2.6	0	0.026823486	0.053505313	0.067642642
2.7	0	0.026486513	0.051714305	0.06586069
2.8	0	0.026150727	0.049933414	0.064088856
2.9	0	0.025816171	0.048162517	0.062327018
3	0	0.025482887	0.046401497	0.060575059
3.1	0	0.025150913	0.044650239	0.058832862
3.2	0	0.024820284	0.042908628	0.057100316
3.3	0	0.024491034	0.041176554	0.055377307
3.4	0	0.024163191	0.039453909	0.053663728
3.5	0	0.023836785	0.037740585	0.051959473
3.6	0	0.023511841	0.036036479	0.050264436
3.7	0	0.023188383	0.034341487	0.048578515
3.8	0	0.022866433	0.03265551	0.04690161
3.9	0	0.022546011	0.030978448	0.045233622
4	0	0.022227135	0.029310207	0.043574456
4.1	0	0.021909823	0.02765069	0.041924015
4.2	0	0.021594091	0.025999805	0.040282208
4.3	0	0.021279952	0.02435746	0.038648943

4.4	0	0.02096742	0.022723567	0.03702413
4.5	0	0.020656507	0.021098037	0.035407682
4.6	0	0.020347224	0.019480785	0.033799512
4.7	0	0.020039579	0.017871724	0.032199536
4.8	0	0.019733583	0.016270773	0.030607671
4.9	0	0.019429242	0.014677849	0.029023834
5	0	0.019126565	0.013092873	0.027447945
5.1	0	0.018825557	0.011515764	0.025879926
5.2	0	0.018526224	0.009946447	0.024319699
5.3	0	0.01822857	0.008384844	0.022767187
5.4	0	0.0179326	0.00683088	0.021222317
5.5	0	0.017638317	0.005284483	0.019685013
5.6	0	0.017345724	0.003745579	0.018155204
5.7	0	0.017054823	0.002214098	0.016632819
5.8	0	0.016765616	0.000689969	0.015117787
5.9	0	0.016478105	-0.000826877	0.013610039
6	0	0.016192291	-0.002336508	0.012109509
6.1	0	0.015908173	-0.003838989	0.010616128
6.2	0	0.015625752	-0.005334387	0.009129831
6.3	0	0.015345027	-0.006822766	0.007650554
6.4	0	0.015065998	-0.00830419	0.006178233
6.5	0	0.014788664	-0.009778722	0.004712806
6.6	0	0.014513023	-0.011246423	0.003254211
6.7	0	0.014239074	-0.012707353	0.001802387
6.8	0	0.013966814	-0.014161574	0.000357274
6.9	0	0.013696241	-0.015609142	-0.001081186
7	0	0.013427353	-0.017050117	-0.002513052
7.1	0	0.013160147	-0.018484556	-0.00393838
7.2	0	0.012894621	-0.019912514	-0.005357227
7.3	0	0.01263077	-0.021334047	-0.006769648
7.4	0	0.012368591	-0.02274921	-0.008175698
7.5	0	0.012108082	-0.024158056	-0.009575431

7.6	0	0.011849238	-0.025560639	-0.0109689
7.7	0	0.011592055	-0.026957011	-0.012356156
7.8	0	0.011336529	-0.028347224	-0.013737252
7.9	0	0.011082656	-0.029731327	-0.015112239
8	0	0.010830432	-0.031109372	-0.016481166
8.1	0	0.010579852	-0.032481408	-0.017844083
8.2	0	0.010330912	-0.033847483	-0.019201039
8.3	0	0.010083606	-0.035207646	-0.020552081
8.4	0	0.009837931	-0.036561943	-0.021897258
8.5	0	0.009593881	-0.037910422	-0.023236615
8.6	0	0.009351451	-0.039253129	-0.024570199
8.7	0	0.009110636	-0.040590109	-0.025898056
8.8	0	0.008871431	-0.041921407	-0.027220231
8.9	0	0.008633831	-0.043247068	-0.028536766
9	0	0.00839783	-0.044567134	-0.029847708
9.1	0	0.008163424	-0.04588165	-0.031153098
9.2	0	0.007930606	-0.047190658	-0.032452979
9.3	0	0.007699371	-0.048494199	-0.033747393
9.4	0	0.007469714	-0.049792316	-0.035036382
9.5	0	0.007241629	-0.051085049	-0.036319987
9.6	0	0.007015111	-0.052372439	-0.037598248
9.7	0	0.006790153	-0.053654525	-0.038871204
9.8	0	0.006566751	-0.054931347	-0.040138896
9.9	0	0.006344898	-0.056202944	-0.041401363
10	0	0.006124589	-0.057469355	-0.042658642
10.1	0	0.005905817	-0.058730617	-0.043910772
10.2	0	0.005688578	-0.059986767	-0.04515779
10.3	0	0.005472866	-0.061237844	-0.046399734
10.4	0	0.005258674	-0.062483883	-0.04763664
10.5	0	0.005045996	-0.06372492	-0.048868543
10.6	0	0.004834828	-0.064960992	-0.050095481
10.7	0	0.004625163	-0.066192134	-0.051317488

10.8	0	0.004416994	-0.06741838	-0.052534599
10.9	0	0.004210317	-0.068639765	-0.053746848
11	0	0.004005126	-0.069856323	-0.05495427
11.1	0	0.003801414	-0.071068087	-0.056156898
11.2	0	0.003599175	-0.072275092	-0.057354765
11.3	0	0.003398405	-0.073477369	-0.058547905
11.4	0	0.003199096	-0.074674951	-0.059736349
11.5	0	0.003001243	-0.075867871	-0.060920131
11.6	0	0.002804841	-0.07705616	-0.062099282
11.7	0	0.002609883	-0.07823985	-0.063273832
11.8	0	0.002416364	-0.079418971	-0.064443814
11.9	0	0.002224277	-0.080593555	-0.065609258
12	0	0.002033616	-0.081763631	-0.066770194
12.1	0	0.001844377	-0.08292923	-0.067926653
12.2	0	0.001656554	-0.084090381	-0.069078663
12.3	0	0.001470139	-0.085247114	-0.070226255
12.4	0	0.001285128	-0.086399458	-0.071369458
12.5	0	0.001101515	-0.087547441	-0.072508299
12.6	0	0.000919294	-0.088691092	-0.073642808
12.7	0	0.000738459	-0.089830439	-0.074773013
12.8	0	0.000559006	-0.09096551	-0.075898942
12.9	0	0.000380927	-0.092096332	-0.077020621
13	0	0.000204217	-0.093222932	-0.078138079
13.1	0	0.0000288709	-0.094345339	-0.079251342
13.2	0	-0.000145117	-0.095463577	-0.080360437
13.3	0	-0.000317753	-0.096577673	-0.081465391
13.4	0	-0.000489042	-0.097687654	-0.082566228
13.5	0	-0.000658989	-0.098793546	-0.083662976
13.6	0	-0.000827602	-0.099895373	-0.084755659
13.7	0	-0.000994884	-0.100993162	-0.085844304
13.8	0	-0.001160841	-0.102086937	-0.086928934
13.9	0	-0.00132548	-0.103176723	-0.088009576

14	0	-0.001488805	-0.104262544	-0.089086252
14.1	0	-0.001650821	-0.105344425	-0.090158989
14.2	0	-0.001811535	-0.10642239	-0.091227809
14.3	0	-0.001970952	-0.107496463	-0.092292736
14.4	0	-0.002129076	-0.108566666	-0.093353795
14.5	0	-0.002285914	-0.109633025	-0.094411008
14.6	0	-0.002441471	-0.11069556	-0.095464399
14.7	0	-0.002595752	-0.111754297	-0.09651399
14.8	0	-0.002748762	-0.112809256	-0.097559804
14.9	0	-0.002900507	-0.113860461	-0.098601863
15	0	-0.003050991	-0.114907933	-0.09964019
15.1	0	-0.003200221	-0.115951695	-0.100674807
15.2	0	-0.003348201	-0.116991769	-0.101705735
15.3	0	-0.003494936	-0.118028176	-0.102732996
15.4	0	-0.003640431	-0.119060936	-0.103756612
15.5	0	-0.003784692	-0.120090073	-0.104776603
15.6	0	-0.003927724	-0.121115606	-0.10579299
15.7	0	-0.004069531	-0.122137556	-0.106805795
15.8	0	-0.00421012	-0.123155944	-0.107815037
15.9	0	-0.004349493	-0.124170791	-0.108820738
16	0	-0.004487658	-0.125182115	-0.109822917
16.1	0	-0.004624618	-0.126189938	-0.110821595
16.2	0	-0.004760379	-0.127194279	-0.111816791
16.3	0	-0.004894946	-0.128195158	-0.112808524
16.4	0	-0.005028322	-0.129192594	-0.113796815
16.5	0	-0.005160514	-0.130186606	-0.114781683
16.6	0	-0.005291526	-0.131177215	-0.115763146
16.7	0	-0.005421363	-0.132164437	-0.116741224
16.8	0	-0.005550029	-0.133148293	-0.117715935
16.9	0	-0.00567753	-0.134128801	-0.118687298
17	0	-0.00580387	-0.135105979	-0.119655331
17.1	0	-0.005929053	-0.136079845	-0.120620054

17.2	0	-0.006053085	-0.137050418	-0.121581483
17.3	0	-0.00617597	-0.138017716	-0.122539636
17.4	0	-0.006297713	-0.138981756	-0.123494532
17.5	0	-0.006418318	-0.139942556	-0.124446188
17.6	0	-0.00653779	-0.140900133	-0.125394622
17.7	0	-0.006656133	-0.141854505	-0.12633985
17.8	0	-0.006773353	-0.142805689	-0.127281891
17.9	0	-0.006889452	-0.143753701	-0.128220761
18	0	-0.007004437	-0.144698559	-0.129156476
18.1	0	-0.007118311	-0.14564028	-0.130089054
18.2	0	-0.007231078	-0.14657888	-0.131018512
18.3	0	-0.007342744	-0.147514375	-0.131944865
18.4	0	-0.007453313	-0.148446782	-0.13286813
18.5	0	-0.007562788	-0.149376117	-0.133788323
18.6	0	-0.007671174	-0.150302395	-0.13470546
18.7	0	-0.007778476	-0.151225634	-0.135619558
18.8	0	-0.007884698	-0.152145848	-0.136530631
18.9	0	-0.007989844	-0.153063053	-0.137438696
19	0	-0.008093918	-0.153977265	-0.138343768
19.1	0	-0.008196924	-0.154888499	-0.139245862
19.2	0	-0.008298867	-0.15579677	-0.140144993
19.3	0	-0.008399751	-0.156702094	-0.141041177
19.4	0	-0.00849958	-0.157604485	-0.141934429
19.5	0	-0.008598358	-0.158503958	-0.142824764
19.6	0	-0.008696089	-0.159400529	-0.143712196
19.7	0	-0.008792777	-0.16029421	-0.144596739
19.8	0	-0.008888426	-0.161185018	-0.14547841
19.9	0	-0.008983041	-0.162072967	-0.146357221
20	0	-0.009076625	-0.16295807	-0.147233187