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Research Article

Study of Hardness of Superhard Crystals by Topological Indices

Xiujun Zhang[1], **Muhammad Naeem**[2], **Abdul Qudair Baig**[2], **and Manzoor Ahmad Zahid**[3]

[1]*School of Computer Science, Chengdu University, Chengdu, China*
[2]*Department of Mathematics and Statistics, Institute of Southern Punjab, Multan, Pakistan*
[3]*Department of Mathematics, COMSATS University Islamabad, Sahiwal, Pakistan*

Correspondence should be addressed to Muhammad Naeem; naeempkn@gmail.com

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Topological indices give immense information about a molecular structure or chemical structure. The hardness of materials for the indentation can be defined microscopically as the total resistance and effect of chemical bonds in the respective materials. The aim of this paper is to study the hardness of some superhard BC_x crystals by means of topological indices, specifically Randić index and atom-bond connectivity index.

1. Introduction

Hardness measures the crystal property of resistance into its deformation. In crystal-type materials, the resistence depends on the chemical bonds between its atoms. In the case of common metals and materials, there exists a delocalized form of bonding. For the domination of the hardness value, the dislocation density which is stored in metals is sufficient. There are many strategies that exist to establish the microscopic theory for the hardness level, and the main ideas are to analyze the experimental material (or metal). There also exist some microscopic hardness models for the prediction of hardness, and these can be applied to covalent (and in some cases to ionic type) crystals (see Gao et al. [1]). A technique to relate the hardness of Vickers for a large class of crystals of covalent type to their microscopic properties has been studied in [2]. To energetically break an electron pair bond has the meaning that two electrons excite from the valence band to the conduction band in covalent crystals. In [3], Gilman proved that the activation energy that is required for a plastic slip is double the band gap denoted as E_g. The force of resistance of a bond can be computed by studying respective E_g of the materials. The form of the hardness for pure covalent-type crystals consists of three variables, and it is formulated as

$$H\,(\text{Gpa}) = AN_aE_g, \tag{1}$$

where A is the constant of proportionality and N_a represents the covalent bond number, and it is per unit area; this area is such that it can be computed from the valence electron density N_e as

$$N_a = \left(\frac{\sum_i n_i Z_i}{2V}\right) = \left(\frac{N_e}{2}\right)^{2/3}, \tag{2}$$

where n_i is the position in the form of a number of the ith atom in the unit cell, Z_i is the valence electron number of the ith atom crediting to the covalent bond, and V is the volume of the unit cell. More results on the hardness (various definitions of hardness) study of crystals can be referred to Suzuki et al. [4], Armstrong et al. [5], Mamun et al. [6], Shkir et al. [7], and Palatnikov et al. [8].

Now, if we talk about the unit crystals studied in this article, then the first one is BC_2, and by the first-principles computations, BC_2 was predicted originally from (a kind of tetragonal phase) the cubic diamond structure. The lattice of the BC_2 structure is tetragonal, and this structure possesses the simple kind of the stacking sequence such as $BC_2BC_2\ldots$ along with the c-axis. Monitoring different states of the electronic densities of BC_2 shows that, in the crystal, all the $B-C$- and $C-C$-type bonds are purely metallic. The known

hardness level of BC_2 is 56 GPa (gigapascal), and this level is very close to that of cubic boron nitride.

Now, compound BC_3 has a different type of crystal structure which is more like and similar to graphite, and so, it has a hexagonal crystal-type structure. A study was performed in [2] to investigate some improved oxidation resistance in a graphitic material that contains very high collections of secondary boron. The procedure to create and find such samples is a reaction between boron trichloride and benzene to examine for chemical composition and crystal structure.

Another class of recently discovered compounds, which has almost the same structure as that of the diamond, is the crystal structure of BC_5. For the purpose of correlation, compound BC_5 is very important, and it is also very useful to know under which type of conditions this compound can be extracted. As a function of pressure, the stability of compound BC_5 is relative to a solution of compound BC_3 and graphite.

Another similar but different compound is the BC_7 crystal structure which is more like to both compound structures of graphite and diamond. By computing the constants of elasticity and frequencies of phonon, the structural stability of the assumed compound crystal structure BC_7 has been confirmed. Similar to the direction for tensile strength of the diamond-like BC_7, its ideal tensile strength was 155.2 GPa; this strength is about 52% more than that of the recent diamond-like predicted structure BC_5. The theoretical Vickers hardness of the diamond crystals like BC_7 was 78 GP_a which indicates that it is a superhard material; these readings show that BC_7 is a superhard material (see in [2]).

We can formulate the Vickers hardness in the form of f_i, N_e, and d as follows:

$$H_v\,(\mathrm{GPa}) = 556\frac{N_a e^{-1.191 f_1}}{d^{2.5}} = 350\frac{N_e^{2/3} e^{-1.191 f_1}}{d^{2.5}}, \tag{3}$$

where f_i is the ionicity of the chemical bond in a crystal scale and d is the bond length in angstroms [9].

In the 70's, one of the famous degree-based indices is the Randić index which was introduced by Randić [10] in 1975, and it is characterized as

$$R_{-(1/2)}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{4}$$

In 1998, Bollobás and Erdos [11] and Amić et al. [12] proposed the general Randić index which is stated as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha. \tag{5}$$

Das et al. [13] studied the relationship between the Randić index and other degree-based indices. Milivojević and Pavlović [14] presented the extremal value and graphs for the variation of the Randić index with regard to minimum and maximum degrees.

Atom-bond connectivity index (in short, ABC index) was introduced by Estrada et al. [15] to measure the stability of alkanes and the strain energy of cycloalkanes which can be formulated by

$$\mathrm{ABC}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{6}$$

Dimitrov [16] provided an affirmative answer of a strengthened version of the previous conjecture and presented that a tree with a minimal ABC index cannot contain a pendent path of length 3 if its order is larger than 415. Dimitrov and Milosavljević [17] manifested several properties of the degree sequences of the trees with minimal ABC index, and a new algorithm for minimal-ABC trees is given. The definitions of more topological indices and results can be referred to Gao et al. [18–22]. Some more literature studies are also available in [23, 24].

The applications of moving correlation coefficient technique enable us to examine the variation in the degree of correlation between correlation stratigraphic sequence and analysis the measure of variables within the framework of a single stratigraphic sequence. Cumulative correlation technique allows to determining more precisely, where such variation took place and it influences every member within the sequence of the preceding ones.

Since both hardness properties and topological indices are important topics in crystal science, it inspired us to study the relationship between them. The main contribution of this paper is to study the hardness of some superhard BC_x crystals in the light of topological indices.

2. Main Results

Many $B-C$ binary systems show high resistance to oxidation and reaction with ferrous metals, compared with the carbon-based materials. In Figure 1, we present selected BC_x systems with specific crystal structures found in [2]. The Randić and atom-bond connectivity indices of these 12 types of BC crystals are computed as follows.

From Figure 1(a), we can see that the number of edges in the unit cell of BC_2/41/amd is 36. We present the edge partition of BC_2/41/amd in Table 1 based on the degree of vertices of each edge. The Randić index and ABC index for the BC_2/41/amd crystal are computed using Table 1, and they are 14.136584 and 25.3452096, respectively.

The number of edges of $BC_3P\bar{4}\,m2$, from Figure 1(b), is 12, and 8 of its edges are of type (1, 3), and 4 are of type (3, 4). This gives us the Randić and ABC indices 5.773502692 and 9.113961545, respectively.

The number of edges in both BC_3Pmmaa and BC_3Pmmab is 12 by Figures 1(c) and 1(d). The edge type of these two structures is also the same, containing 4 edges of type (1, 3), 2 edges of type (3, 3), 4 edges of type (2, 3), and 2 edges of type (2, 2). So, the Randić and ABC indices of BC_3Pmmaa and BC_3Pmmab are the same. They are 5.6090609 and 8.84196034, respectively.

From Figure 1(e), we can see that $BC_5I\bar{4}\,m2$ consists of 20 edges. The degree-based edge partition of this structure is given by 10 edges of type (2, 2), 8 edges of type (2, 3), and 2

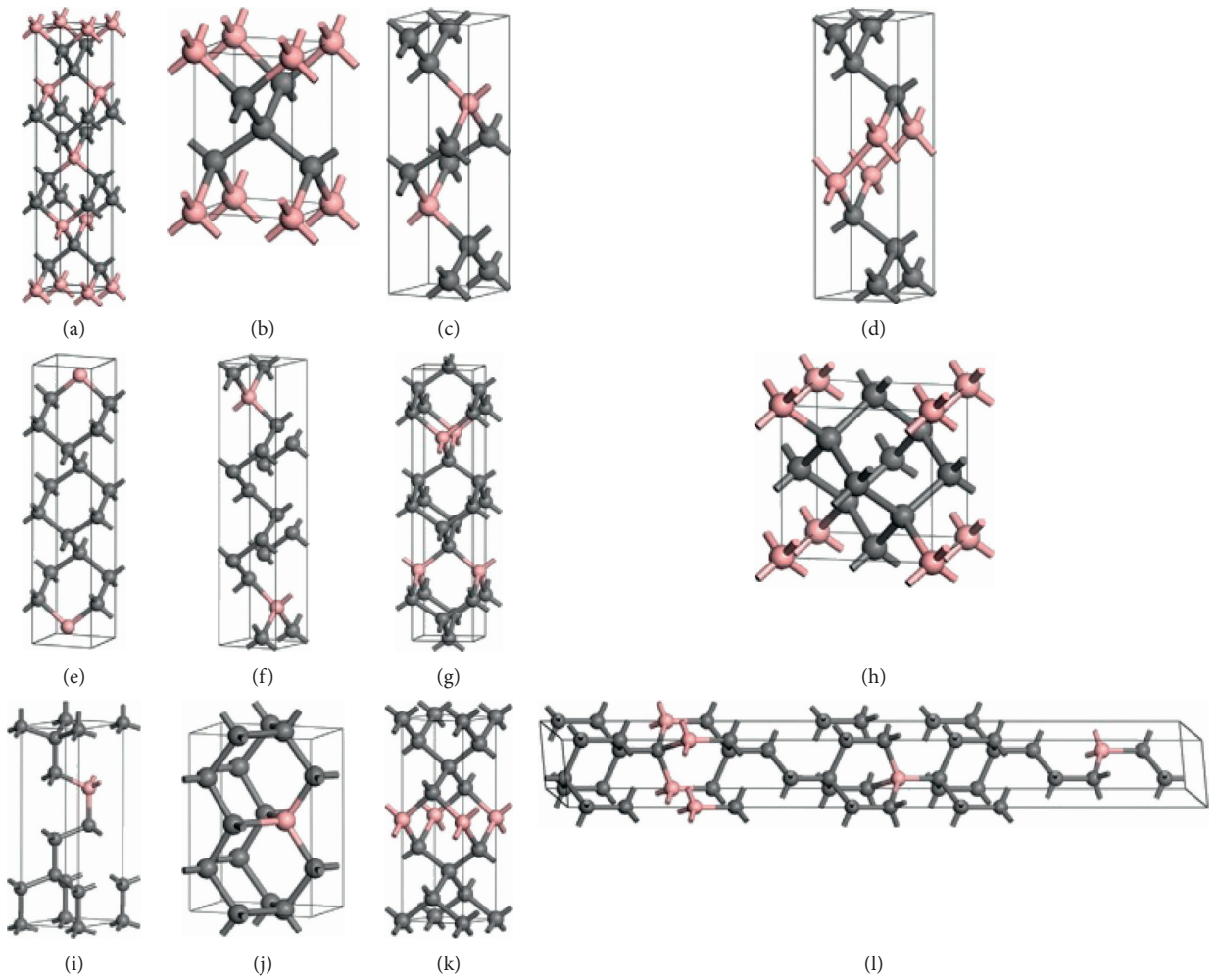

Figure 1: Crystal structures of (a) BC_2I41/amd, (b) BC_2P4m2, (c) BC_3Pmma-a, (d) BC_3Pmma-b, (e) BC_5I41/amd, (f) BC_5Pmma-1, (g) BC_5Pmma-2, (h) $BC_7P\bar{4}$ 3m, (i) BC_7P3m1, (j) BC_7Pmm2, (k) BC_7P4m2, and (l) BC_7R3m. Boron atoms are shown in orange.

Table 1: Edge partition of BC_2I41/amd.

d_u, d_v	Frequency
(1, 3)	8
(2, 3)	12
(3, 4)	16

edges of type (3, 3). This gives us the Randić and ABC indices as 8.93265299 and 14.0612554, respectively.

The number of edges of BC_5Pmma1, from Figure 1(f), is 15. Its degree-based edge partition is given by 4 edges of type (1, 3), 2 edges of type (2, 3), 2 edges of type (1, 1), and 7 edges of type (2, 2). So, the Randić and ABC indices are 12.4282032 and 9.62994735, respectively.

The number of edges of BC_5Pmma2, from Figure 1(g), is 36. Its degree-based edge partition contains 4 edges of type (2, 3), 24 edges of type (3, 3), and 8 edges of type (3, 4). So, the Randić and ABC indices are 11.9423942 and 23.9924049, respectively. From Figure 1(h), the number of edges of $BC_7P\bar{4}$ 3m is 16. Its degree-based edge partition contains 4 edges of type (1, 4) and 12 edges of type (2, 4). So, the Randić and ABC indices for this crystal are 6.24264069 and 11.949383, respectively.

The number of edges of BC_7P3m1, from Figure 1(i), is 15. Its degree-based edge partition is given by 1 edge of type (1, 1), 3 edges of type (1, 2), 5 edges of type (2, 4), 3 edges of type (1, 4), and 3 edges of type (2, 3). So, the Randić and ABC indices are 7.61383217 and 10.3762508, respectively. From Figure 1(j), the number of edges of is 18. BC_7Pmm2 Its degree-based edge partition is given by 12 edges of type (2, 3), 2 edges of type (3, 3), and 4 edges of type (2, 2). So, the Randić and ABC indices are 7.56564615 and 12.6470418, respectively.

The number of edges of BC_7P4m2, from Figure 1(k), is 24. Its degree-based edge partition contains 8 edges of type (1, 3), 8 edges of type (3, 4), and 8 edges of type (2, 3). So, the Randić and ABC indices are 10.1941896 and 17.3528047, respectively. From Figure 1(l), the number of edges of BC_7R3m is 51. Its degree-based edge partition contains 2

Table 2: Hardness (H) of crystals BC_2I41/amd, BC_3P4m2, BC_3Pmmma-a, BC_3Pmmma-b, BC_5I41/amd, BC_5Pmmma-1, BC_5Pmmma-2, $BC_7P\bar{4}3m$, BC_7P3m1, BC_7Pmm2, BC_7P4m2, and BC_7Pmm2.

Crystal	Symmetry	Hardness	Reference
BC_2	$I4_1/amd$	56	[28]
BC_3	$P\bar{4}m2$	65.8	[26]
	$Pmma-a$	61.9	[26]
	$Pmma-b$	64.8	[26]
BC_5	$I\bar{4}m2$	80	[30]
	$Pmma-1$	74	[25]
	$Pmma-2$	70	[25]
BC_7	$P\bar{4}3m$	77.6	[29]
	$P3m1$	65.3	[27]
	$Pmm2$	80.7	[27]
	$P\bar{4}m2$	75.2	[27]
	$R3m$	65.4	[27]

Table 3: Structure symmetry, Randić index (R), atom-bond connectivity (ABC) index, calculated hardness (H), and their cumulative correlations (Cor) between (R, H) and (ABC, H).

Crystal	Symmetry	Randić index (R)	ABC index	Hardness of crystals	Cor (R, H)	Cor (ABC, H)
BC_2	$I4_1/amd$	14.136584	25.3452096	56.0	—	—
BC_3	$P\bar{4}m2$	5.77350269	9.11396154	65.8	−1	−1
	$Pmma-a$	5.6090609	8.84196034	61.9	−0.911790078	−0.9128016
	$Pmma-b$	5.60906090	8.84196034	64.8	−0.921902798	−0.92264538
BC_5	$I\bar{4}m2$	8.93265299	14.0612554	80.0	−0.267918644	−0.33848122
	$Pmma-1$	12.4282032	9.62994735	74.0	−0.028477805	−0.39185327
	$Pmma-2$	11.9423942	23.9924049	70.0	0.019298886	−0.23407776
BC_7	$P\bar{4}3m$	6.24264069	11.949383	77.6	−0.11272915	−0.26114031
	$P3m1$	7.61383217	10.3762508	65.3	−0.092422184	−0.2263985
	$Pmm2$	7.56564615	12.6470418	80.7	−0.134370355	−0.22184915
	$P\bar{4}m2$	10.1941896	17.3528047	75.2	−0.096163473	−0.17150281
	$R3m$	22.8743687	34.3374432	65.4	−0.197758916	−0.24340232

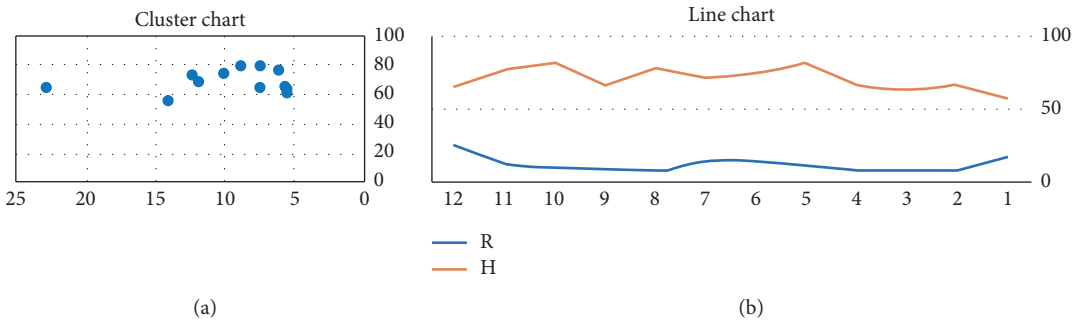

Figure 2: Cluster and line chart of R and H.

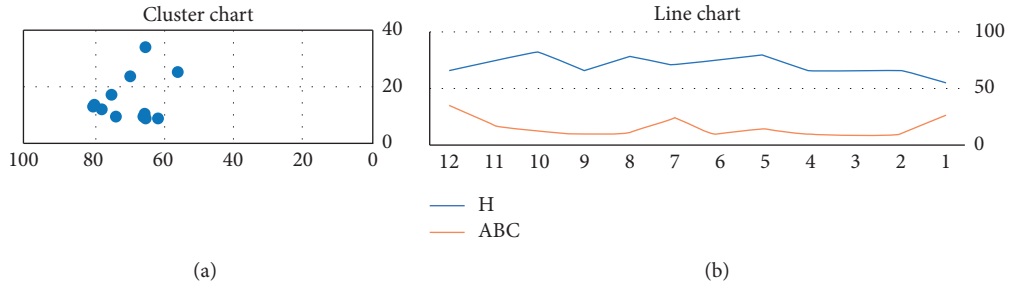

Figure 3: Cluster and line chart of ABC and H.

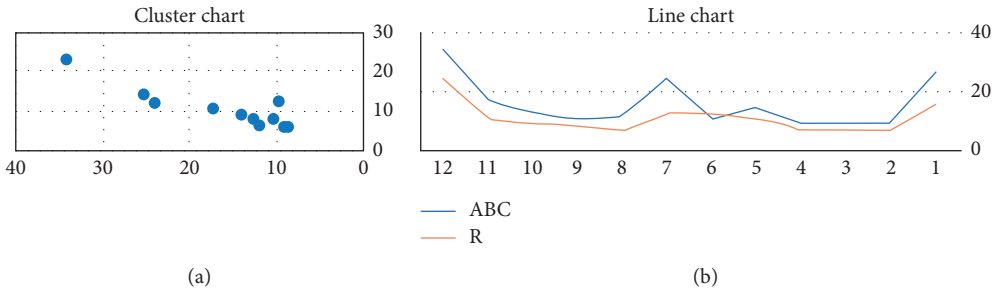

Figure 4: Cluster and line chart of R and ABC.

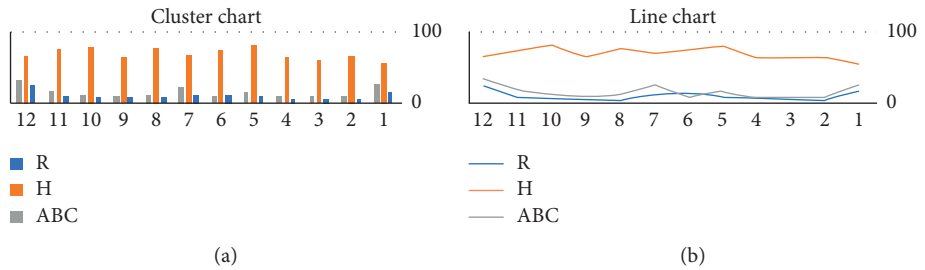

Figure 5: Cluster and line chart of ABC, R, and H.

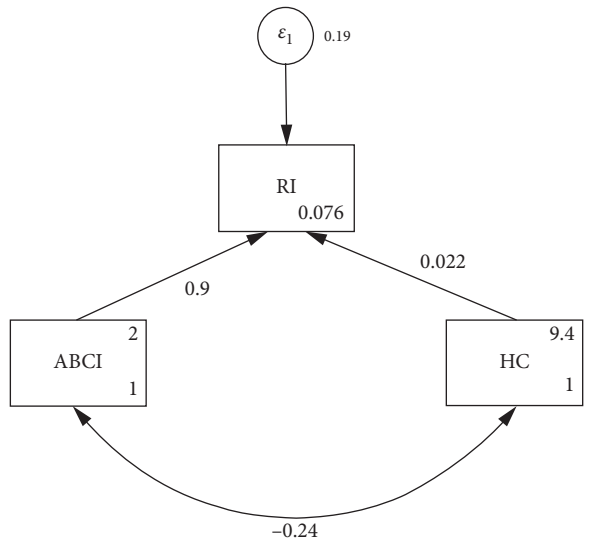

Figure 6: The magnitude of the effectiveness of ABCI and HC over RI.

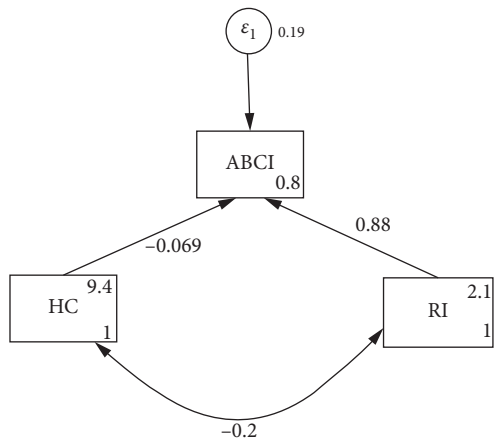

Figure 7: The magnitude of the effectiveness of RI and HC over ABCI.

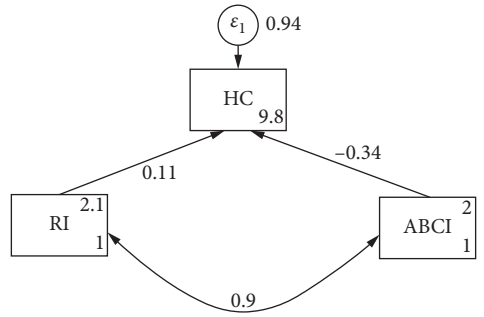

Figure 8: The magnitude of the effectiveness of ABCI and RI over HC.

SEM

Endogenous variables

Observed : RI

Exogenous variables

Observed : ABCI HC

Fitting target model :

Iteration 0 : log likelihood = −108.5116
Iteration 1 : log likelihood = −108.5116

Structural equation model — Number of obs = 12
Estimation method = *m*1
Log likelihood = −108.5116

Standardized	OIM Coef.	Std. Err.	*z*	$P > \|z\|$	[95% conf.	interval]
Structural						
RI <-						
ABCI	0.9025842	0.0636826	14.17	0.000	0.7777685	1.0274
HC	0.0219322	0.1313459	0.17	0.867	−0.2355011	0.2793655
_cons	0.0757925	1.32599	0.06	0.954	−2.523101	2.674686
Mean (ABCI)	1.978639	0.4964462	3.99	0.000	1.005622	2.951655
Mean (HC)	9.373905	1.935094	4.84	0.000	5.581191	13.16662
Var (e.RI)	0.1944974	0.1007828			0.0704443	0.5370088
Var (ABCI)	1	.			.	.
Var (HC)	1	.			.	.
Cov (ABCI, HC)	−0.2434024	0.2715727	−0.90	0.370	−0.775675	0.2888702

LR test of model vs. saturated: chi^2 (0) = 0.00, prob > chi^2 = .

Figure 9: Tabular form of the magnitude of the effectiveness of ABCI and HC over RI as shown in Figure 6.

Endogenous variables

Observed : ABCI

Exogenous variables

Observed : HC RI

Fitting target model :

Iteration 0 : log likelihood = –108.5116
Iteration 1 : log likelihood = –108.5116

Structural equation model Number of obs = 12
Estimation method = *m*1
Log likelihood = –108.5116

Standardized	OIM Coef.	Std. Err.	*z*	*P* > |*z*|	[95% conf.	interval]
Structural						
ABCI <-						
HC	–0.0686487	0.1293607	–0.53	0.596	–0.3221911	0.1848937
RI	0.88367	0.0664661	13.30	0.000	0.7533988	1.013941
_cons	0.7953603	1.311625	0.61	0.544	–1.775377	3.366097
Mean (HC)	9.373905	1.935094	4.84	0.000	5.581191	13.16662
Mean (RI)	2.067271	0.5112733	4.04	0.000	1.065194	3.069348
Var (e.ABCI)	0.1904215	0.0989202			0.0687914	0.5271064
Var (HC)	1	.			.	.
Var (RI)	1	.			.	.
Cov (HC, RI)	–0.197759	0.2773855	–0.71	0.476	–0.7414245	0.3459065

LR test of model vs. saturated: chi^2 (0) = 0.00, prob > chi^2 = .

Figure 10: Tabular form of the magnitude of the effectiveness of RI and HC over ABCI as shown in Figure 7.

Endogenous variables

Observed : HC

Exogenous variables

Observed : RI ABCI

Fitting target model :

Iteration 0 : log likelihood = –108.5116
Iteration 1 : log likelihood = –108.5116

Structural equation model — Number of obs = 12
Estimation method = *m*1
Log likelihood = –108.5116

Standardized	OIM Coef.	Std. Err.	*z*	$P > \|z\|$	[95% conf.	interval]
Structural						
HC <-						
RI	0.1058366	0.6327297	0.17	0.867	–1.134291	1.345964
ABCI	–0.3383638	0.6263131	–0.54	0.589	–1.565915	0.8891874
_cons	9.824612	1.935909	5.07	0.000	6.030301	13.61892
Mean (RI)	2.067271	0.5112733	4.04	0.000	1.065194	3.069348
Mean (ABCI)	1.978639	0.4964462	3.99	0.000	1.005622	2.951655
Var (e.HC)	0.9385716	0.1343048			0.7090303	1.242424
Var (RI)	1	.			.	.
Var (ABCI)	1	.			.	.
Conv (RI, ABCI)	0.8972459	0.0562772	15.94	0.000	0.7869446	1.007547

LR test of model vs. saturated: chi^2 (0) = 0.00, prob > chi^2 = .

Figure 11: Tabular form of the magnitude of the effectiveness of ABCI and RI over HC as shown in Figure 8.

edges of type (1, 1), 5 edges of type (1, 2), 14 edges of type (2, 2), 2 edges of type (4, 4), 25 edges of type (2, 4), and 3 edges of type (3, 3). So, the Randić and ABC indices for this crystal are 22.8743687 and 34.3374432, respectively.

In [25–30], Li et al., Liu et al., L. Xu et al., and Yao et al. computed the hardness of the above selected crystals shown in Figure 1. The hardness of all the crystals is given in Table 2.

Table 3 shows the crystal structures of Figure 1 along with their Randić index (R), atom-bond connectivity (ABC) index, calculated hardness (H) from Table 2, and cumulative correlations (Cor) between (R, H) and (ABC, H).

3. Comparison

In this section, we have compared the hardness of subjected materials with Randic and ABC indices. Figure 2 shows the comparison between the Randic index and hardness of the subjected materials given in Table 3. Figure 3 shows the comparison between the ABC index and hardness.

Figure 4 shows the comparison between the Randic index and ABC index of the subjected materials given in Figure 1.

Figure 5 shows the comparison between the hardness, Randic index, and ABC index of the subjected materials given in Figure 1.

4. Conclusion and Discussion

We have investigated the association among the Randić index (RI), hardness of the crystal (HC), and atom-bond connectivity index (ABCI). For this purpose, the structural equation model (SEM) has been applied by the structure of three equations. Figures 6–8 show us the magnitude of the effectiveness of ABCI and HC over RI, of RI and HC over ABCI, and of ABCI and RI over HC, respectively. Figures 9–11 give us the tabular form of the magnitude of the effectiveness of ABCI and HC over RI as shown in Figure 6, of RI and HC over ABCI as shown in Figure 7, and of ABCI and RI over HC as shown in Figure 8, respectively. Estimates of three equations depict that ABCI is positively and significantly associated with RI, and 1 unit increase in ABCI improves 0.90 units of RI, while HC is positively and insignificantly related with RI. Negative and insignificant magnitude of HC is observed with ABCI. However, RI is positively and significantly related with ABCI. Contradictory results are observed about the impact of RI and ABCI on HC; both RI and ABCI are insignificantly linked with HC. In this article, we have started a new study which relates the hardness and topological indices of superhard crystals; which can contribute to some futuristic applications, and we encourage others to do more research in this area.

Data Availability

All the data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

All the authors contributed equally to this study. M. Naeem and A. Q. Baig completed all the computations, wrote the manuscript, and added all figures. X. Zhang checked and corrected the initial manuscript. M. A. Zahid added some final remarks and improved the overall paper. All authors read and approved the final draft.

Acknowledgments

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