

Mode: Similarity Report

sources:

1 1,018 words / 15% - CrossCheck
[Goudarz Mohseni Rouzbehani. "B24N24 nanocages: a GIAO density functional theory study of 14N and 11B nuclear magnetic shielding and electric field gradient tensors", Monatshefte für Chemie - Chemical Monthly, 03/2009](#)

2 240 words / 3% - CrossCheck
[Domingo, L.R.. "A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies", Chemical Physics Letters, 20070420](#)

3 116 words / 2% - Internet from Apr 2, 2010
www.mdpi.com

4 83 words / 1% - Publications
[Boshra, Asadollah Seif, Ahmad. "A boroxol ring doped zigzag boron nitride nanotube: a computational DFT study of the quadrupole coup", Canadian Journal of Physics, June 2009 Issue](#)

5 73 words / 1% - Internet from May 10, 2011
iaub.iau.ofis.ir

6 68 words / 1% - CrossCheck
[Hai-Shun Wu. "The structure and stability of B36N36 cages: a computational study", Journal of Molecular Modeling, 12/2005](#)

7 67 words / 1% - CrossCheck
[Nima Karachi. "DFT based insights into reactivity descriptors of encapsulated B24N24 nanocages", Structural Chemistry, 02/24/2011](#)

8 62 words / 1% - CrossCheck
[Jeschke, G.. "A comprehensive NMR study of cubic and hexagonal boron nitride", Solid State Nuclear Magnetic Resonance, 199808](#)

9 50 words / 1% - CrossCheck
[Seif, A.. "Lithium-doped \(4,4\) Boron nitride nanotube: Density functional theory study of N and B](#)

10

41 words / 1% - Internet from Jun 6, 2011
epubs.cclrc.ac.uk

11

35 words / 1% - Internet from Oct 26, 2011
www.jnsc.ir

12

34 words / < 1% match - CrossCheck
[Latosinska, J.. "The tautomeric equilibria of cytosine studied by NQR spectroscopy and HF, MP2 and DFT calculations". Journal of Molecular Structure, 20030312](#)

13

33 words / < 1% match - CrossCheck
[M. A. Mileev. "Ab initio calculations of structure and stability of small boron nitride clusters". Journal of Structural Chemistry, 11/2006](#)

14

32 words / < 1% match - CrossCheck
[Farahani, M.. "A DFT study of the nuclear magnetic response of the zigzag AIN-BN and BN-AIN nanotube junctions", Journal of Molecular Structure: THEOCHEM, 20091115](#)

15

31 words / < 1% match - CrossCheck
[Nirmala, V.. "Structure and electronic properties of armchair boron nitride nanotubes". Journal of Molecular Structure: THEOCHEM, 20070901](#)

16

29 words / < 1% match - CrossCheck
[Mirzaei, M.. "Density functional calculations of \$^{14}\text{N}\$ and \$^{10}\text{B}\$ NQR parameters in the H-capped \(6,0\) and \(4,4\) single-walled BN nanotubes", Physica E: Low-dimensional Systems and Nanostructures, 200802](#)

17

27 words / < 1% match - CrossCheck
[Nishiwaki, A.. "Atomic structures and stability of boron nitride nanotubes with a cup-stacked structure", Diamond & Related Materials, 200503/07](#)

18

24 words / < 1% match - CrossCheck
[Brasca, R.. "Theoretical explanation of the regioselectivity of polar cycloaddition reactions between furan derivatives and Danishefsky's diene". Journal of Molecular Structure: THEOCHEM, 20091015](#)

19

20 words / < 1% match - Internet from Jan 23, 2011
utopia.uv.es

20

19 words / < 1% match - CrossCheck

[Seif, A.. "Density functional calculations Al-27 and N-14 quadrupole coupling constants in the H-capped \(10,0\) and \(4,4\) single-walled aluminum nitride nanotube". Journal of Molecular Structure: THEOCHEM, 20080815](#)

21

18 words / < 1% match - Internet from May 25, 2009

cornwallinquiry.irri.net

22

17 words / < 1% match - Internet from Jun 17, 2008

www.physics.wm.edu

23

17 words / < 1% match - CrossCheck

[Zope, R.R.. "Electronic structure, vibrational stability, infra-red, and Raman spectra of B²N²4 cages". Chemical Physics Letters, 20040801](#)

24

15 words / < 1% match - CrossCheck

[Zahedi, E.. "The influence of NH³-attaching on the NMR parameters in the zigzag BN nanotube". Superlattices and Microstructures, 201102](#)

25

15 words / < 1% match - CrossCheck

[Mahmoud Mirzaei. "Computational NQR study of a boron nitride nanocone", Monatshefte für Chemie - Chemical Monthly, 02/12/2010](#)

26

15 words / < 1% match - CrossCheck

[Jung, J.K.. "NMR study of boron nitride nanotubes". Solid State Communications, 200404](#)

27

14 words / < 1% match - CrossCheck

[Oliaey, A.R.. "Spin polarized bonding analysis of endohedral boron nitride nanocages: Density functional theory study", Physica E: Low-dimensional Systems and Nanostructures, 201007](#)

28

12 words / < 1% match - Internet from May 8, 2003

www.ijms.org

29

12 words / < 1% match - CrossCheck

[Seif, A.. "A DFT studies of structural and quadrupole coupling constants properties in C-doped BeO nanotubes". Superlattices and Microstructures, 201111](#)

30

11 words / < 1% match - Internet from Jul 7, 2008

znaturforsch.com

31

11 words / < 1% match - Internet from Feb 18, 2010

www.iop.org

32

9 words / < 1% match - Internet from Aug 19, 2010

www.waset.org

33

9 words / < 1% match - Internet from Sep 25, 2008

chemistry.hanyang.ac.kr

34

8 words / < 1% match - CrossCheck

[Mahmoud Mirzaei. "SiC-doped boron nitride nanotubes: computations of 11B and 14N quadrupole coupling constants", Monatshefte für Chemie - Chemical Monthly, 04/09/2010](#)

35

8 words / < 1% match - CrossCheck

[V. NIRMALA. International Journal of Nanoscience, 2005](#)

36

8 words / < 1% match - CrossCheck

[Pokropivny, V.V.. "Boron Nitride Analogs of Fullerenes \(the Fulborenes\), Nanotubes, and Fullerites \(the Fulborenites\)", Journal of Solid State Chemistry, 200010](#)

37

8 words / < 1% match - CrossCheck

[Kato, T.. "The essential role of the electronegativity perturbation in vibronic interactions in positively charged B,N-substituted acenes", Chemical Physics, 20050808](#)

38

8 words / < 1% match - CrossCheck

[Izadyar, M.. "Kinetics and mechanism of 2-pyridylacetic acid pyrolysis in the gas phase: A joint experimental and theoretical study", Chemical Physics, 20061121](#)

39

8 words / < 1% match - CrossCheck

[Xiaojun Wu. "Adsorption of transition-metal atoms on boron nitride nanotube: A density-functional study", The Journal of Chemical Physics, 2006](#)

40

7 words / < 1% match - CrossCheck

["Master Index", Journal of Molecular Structure: THEOCHEM, 20011221](#)

41

6 words / < 1% match - CrossCheck

[Khodaei, S.. "Theoretical investigation of hydrogen bonding effects on oxygen, nitrogen, and hydrogen chemical shielding and electric field gradient tensors of chitosan/HI salt", Carbohydrate Research, 20071126](#)

42

6 words / < 1% match - CrossCheck

[Rai, A.K.. "Conformational search for zwitterionic leucine and hydrated conformers of both the canonical and zwitterionic leucine using the DFT-CPCM model", Vibrational Spectroscopy, 20110512](#)

43

6 words / < 1% match - CrossCheck

[Borst, D.R.. "Hydrogen bonding and tunneling in the 2-pyridone.2-hydroxypyridine dimer. Effect of electronic excitation". Chemical Physics. 20021001](#)

44

6 words / < 1% match - CrossCheck

[L. V. Stankevich. "Polyhedral boron nitride molecules", Russian Chemical Bulletin, 10/1993](#)

paper text:

Journal of Nanostructure in Chemistry 2 (2) (2011) 98-109 Contents list available at JNSC Journal of Nanostructure in Chemistry (JNSC) I.A.U. journal homepage: www.jnsc.ir

DFT study of nuclear magnetic shielding, electric field gradient tensors and electrophilicity indices of Magic BN nanocages

11

a,* b cd e

Asadollah Boshra , Siamak Jadidi , Ahmad reza Oliaey , Majid

11

Monajjemi , Mehran Aghaie a, *

**Nanoscience Computation Lab, Islamic Azad University, Boroujerd Branch, Boroujerd, Iran.
P.O.Box 6915136111.**

7

Tel.

0098-662-4453000. Fax. 0098-662-4453013. Email: [a.boshra@](mailto:a.boshra@iaub.ac.ir)

32

iaub.ac.ir. b

Department of Physics, Science and Research Branch, Islamic Azad University, Hesarak,
Tehran, Iran, P.O. Box 14515-775.

7

Tel. 0098-21-44865016, Fax 0098-44817175. Email: jadidisiamak@yahoo.com c

Department of Chemistry, Tonekabon branch, Islamic Azad University, Tonekabon, Iran,
P.O.Box 14515-775.

27

Tel. 0098-192-4271106. Fax : 0098-192- 4274409. Email: a_oliyayi@tonekaboniau.ac.ir d

Department of Chemistry, Science and Research Branch, Islamic Azad University, Hesarak,
Tehran, Iran, P.O. Box 14515-775.

7

Tel. 0098-21-44865016, Fax 0098-44817175. Email: m_monajjemi@yahoo.com e

Faculty of Chemistry, North Tehran Branch, Islamic Azad University, Tehran, Iran.

30

Tel. 0098-21-2226256. Email: marmin2004200@yahoo.com. ARTICLE INFO Article history: Received 20 January 2011
Accepted 2 April 2011 Keywords: Magic BN nanocages, Density functional theory, Nuclear magnetic shielding, Electron
field gradient, GIAO, Electrophilicity index A B S T R A C T

Nuclear magnetic shielding and electric field gradient tensors calculations of the
magic BN

11

fullerenes were performed by DFT method that

employed the Gaussian 98 software implementation of the

5

GIAO method. The calculated NMR parameters provide

a way to identify these nanocages. The NQR parameters

5

are also discussed. All of the results were compared to experimental and theoretical data of related compounds. The electrophilicity index, ω , of magic BN nanocages

has been evaluated from the ionization potential (IP) and the electron affinity (EA) computed by vertical ionization at the B3LYP/

19

6-311++g(d,p) level.

42

*Corresponding author: Asadollah Boshra, Email: a.boshra@gmail.com 99 A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011)

1. Introduction Since the discovery of carbon nanotubes (CNTs) by Iijima [1] in 1991,

29

researches in many areas of physics and chemistry on carbon nanotube (CNT) have reached a critical mass.

Carbon-based nanocage structures, such as fullerene clusters, nanotubes, nanocapsules, nanopolyhedrals, cones, cubes and onions, have wonderful potential for studying materials of low dimensions in an isolated environment [2,3]. In contrast to carbon fullerenes (C

17

and 60 C), there is no direct evidence for the most favored 70 structures of BN analogues, despite advanced synthesis and characterization

6

[4–13].

While the stability of carbon fullerenes is governed by the isolated pentagon rule (IPR), i.e., the

6

maximal and perfect separation of the strained pentagons, the stability of (BN) can be estimated by the isolated n square rule (ISR), i.e., the maximal and perfect separation of the strained squares.

Fowler et al. found that $B_{12}N_{12}$, $B_{16}N_{16}$ and $B_{28}N_{28}$ stand out as "magic" BN fullerenes [14].

Successful attempts to synthesize nanosized structures from boron nitride molecules [15-

13

20] and the development of procedures for the synthesis of pure boron-nitride nanotubes

[21] have stirred the growing interest in calculation of BN structures:

B_nN_n [22], B_nN_n ($n = 0-3$), $B_{12+3n}N_{12+3n}$ and

B_nN_n [23], B_nN_n and B_nN_n [24, 25], B_nN_n

24

$B_{22}N_{22}$, $B_{12}N_{12}$, $B_{16}N_{16}$, $B_{28}N_{28}$ [26],

B_nN_n [27], B_nN_n , B_nN_n and B_nN_n

35

[28], $B_{36}N_{36}$, $B_{12}N_{12}$, $B_{24}N_{24}$, $B_{60}N_{60}$, B_nN_n ($n = 8-33$) [29], B_nN_n ($x = 1-4, 12, 15, 30$) $n = n+4$, $x = x$ [30], ($x = 13, 14, 16$) [31], ($x = 12, 16, 18, 24, 36, 60$) [32], and B_nN_n as a formal analog of Buckminster 30 30 fullerene. Nanocage clusters of BN were synthesized,

and detected by laser desorption time-of-flight mass spectrometry [33]. The

31

self-consistent density functional tight-binding (DFTB) method

40

were employed to investigate atomic and electronic structures and thermal stability of BN nanopeapods ($B_nN_n @BN-NT$)

[34]. Matxain research crew [35] 12 12 were used SIESTA code with the GGA-PBE density functional method to analyze the possibility of assembling of B N fullerenes in molecular solids. 12 12

Sheichenko et al [36] have studied the electronic properties of B_nN_n (n = 12, 24, 60) fullerene-like molecules using semiempirical and ab initio methods. The third-order nonlinear optical polarizabilities for

1

B₁₂N₁₂, B₂₄N₂₄ and B₆₀N₆₀ clusters were

36

calculated 12 12 24 24 36 36

by employing ab initio time-dependent density functional theory combined with a sum-over-states method (SOS//TDDFT)

1

[37]. Shevlin et al [38] were studied the

properties and defects in some nitride (III-V) nanoscale cage clusters

10

(BN, AlN, GaN and, InN) via Density Functional Theory. They found that

the relative stability of different BN clusters has been further explored by studying principal point defects and their complexes including topological B-N bond rotational defects, vacancies, antisites and, interstitials. The

10

calculation of nuclear magnetic resonance (NMR) parameters using ab initio and DFT techniques has become a major method in the investigation of molecular structure.

3

Jung et al[39] were studied 11 B

NMR and the spin lattice relaxation times (T₁) in

26

boron nitride nanotubes to decompose and identify

hexagonal and rhombohedral phases in the BNNTs.

26

14 It has been proved that N

NQR spectra can provide sufficient information to infer about the tautomeric form of a compound

14

12

and,

N NQR frequencies, closest to the experimental ones, can be obtained by the DFT method with Becke B3LYP functional

12

[40]. A. Boshra et al [41] investigated the

nanotube length effect on the aromaticity and CSI parameters of finite length single-wall zigzag and armchair boron nitride nanotubes

5

through DFT framework. A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 100 Also Seif et al [42] in a DFT calculation research showed that how the Li dopant atoms affect NMR and NQR parameters of H

-capped (4,4) single- walled boron nitride nanotube. Moreover, Boshra and

5

his coworkers [43] were presented doping effect

of Boroxol ring on the N-15 and B-11 NMR parameters in zigzag boron nitride nanotube in a 5

density functional theory research. The GIAO DFT study of B N nanocages were carried out to 24 24 evaluate

N and B nuclear magnetic shielding and electric field gradient tensors

5

[44].

We are interested in utilizing DFT computational techniques to look at how variations in the 1
molecular 11 15 structure impact the resulting B and N NMR 11 14 and

also B and N NQR observables, and the electrophilicity index, ω , of magic BN nanocages.

Magnetic nuclei chemical shielding tensors for 11 15 nuclei with fractional spin like B 1
and N reveal very valuable information about the physical environment and especially the
electrostatic environment around the nuclei. However, because of the complex electrostatic
environment of the nanocages, practical spectrometry that directly explores the electrostatic
environment around the nucleus is difficult. Therefore, quantum calculations play a very important
position in measuring the NMR parameters of nanocages. Nuclear quadrupole resonance (NQR)
spectroscopy, which is applied to quadrupole nuclei, is among the most versatile and insightful
techniques used to investigate the physical properties of matter [45]. Quadrupole nuclei are those
that have nuclear spin angular momentum 11 14 greater than one-half ($I > 1/2$), e.g., B and N.

The quadrupole coupling constant (c) and the asymmetry parameter (h) can be determined via
quantum chemical calculations of the electric field gradient (EFG) tensors. c is proportional to the
interaction energy between the nuclear electric quadrupole moment (eQ) and the EFG tensors at the
quadrupole nuclei sites [46]. Another important measurable parameter is the asymmetry parameter
(h), meaning the deviation of the EFG tensors from cylindrical symmetry at quadrupole nuclei sites.
The EFG tensors are very sensitive to the electrostatic environment and can reveal new aspects of
these properties in magic BN fullerenes. Computationally, the calculated EFG tensors are
proportional to c and h; therefore, quantum chemical calculations permit the evaluation of

parameters measurable with NQR. The present computational work investigates the electrostatic properties of magic BN fullerenes systematically. Therefore, the

total electronic energy and HOMO- LUMO energy gap (Table 1) and the

nuclear magnetic shielding tensors and the EFG tensors were calculated in order to evaluate the NMR (s) and NQR iso parameters c and h (Tables

1

2, 3, 4 and 5, 6, 7) of B and N nuclei

as a first prediction for magic BN fullerenes (Figures 1, 2

1

and 3).

Table 1. The total electronic energy E (Hartree) and the

23

a HOMO–LUMO gap (eV) of the of magic BN fullerenes Structure E Energy gap B 12 N 12 -956.349 6.75 B 16 N 16 -1275.305 6.29 B 28 N 28 -2232.148 6.80

In the present Letter, the electrophilicity index, ω , of

2

threeBNnanocages,

B N 2, B N and B N

44

12 1 16 16 28 28

is evaluated from the IP and EA values computed by vertical ionization at the B3LYP/

2

6-311++g(d,p) level (Table

41

8). a See figures 1, 2 and 3 for more details. . 101 A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011)

Figure 1. 3D views of B N magic BNfullerene 12 12 Figure 2. 3D views of B N magic BN fullerene 16 16

are influenced by the structural changes. To the best of our knowledge, no experimental data are currently available on

1

σ or c values and the electrophilicity iso index, ω ,

for the considered clusters in the literature; therefore, the present work evaluates

20

the nuclear magnetic shielding (s), quadrupole coupling iso constant parameters (c) and electrophilicity index, ω ,

as a first prediction for the magic fullborenes.

1

The calculated NQR parameters compare with some experimental results of related compounds.

Table 3. GIAO chemical shieldings (s) of optimized a,

1

b structure of B16N 16 cage (in ppm) Figure3. 3D views of B N magic BN fullerene 28 28 Table 2. GIAO chemical shieldings of optimized structure Boron Nitrogen Atom no. Isotropic Anisotropic Atom no. Isotropic Anisotropic 1 2 3 4 9 12 14 16 17 20 22 24 64 64 64 64 64 64 64 64 64 64 64 64 64 64 64 64 64 a,b of B12N 12 cage (in ppm) 43 43 44 43 44 44 44 44 44 43 43 43 The NMR and NQR parameters indicate

how the electronic structure properties of these BN cages

1

5 6 7 8 10 11 13 15 18 19 21 23 107 107 107 107 107 107 107 107 107 107 107 107 107 142 142 141 142 142 141 142 142
141 141 142 142 Boron Nitrogen Atom no. Isotropic Anisotropic Atom no. Isotropic Anisotropic 1 2 3 4 5 6 7 8 17 20 21
24 27 28 29 32 66 66 68 68 66 66 66 66 66 66 66 66 68 68 66 66 41 42 39 39 41 41 42 41 41 41 41 41 39 39 41 42 9 10
11 12 13 14 15 16 18 19 22 23 25 26 30 31 2. Computational methods 93 93 93 93 130 93 130 93 93 93 94 94 131 131
93 93 147 147 147 147 180 147 180 147 147 147 146 146 179 180 147 147

The quantum chemical calculations at the level of density functional theory were performed on the 16

magic BN fullerenes: B12N 12 (Fig. 1), B16N 16 (Fig. 2) and B28N 28 (Fig. 3) clusters using the Gaussian 98 a See figures 1 and 4 for more details. b Compare the data with the results of [41-44] a See figures 2 and 5 for more details. b Compare the data with the results of [41-44] A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 102 [47] package of program. Table 4. GIAO chemical shieldings (s) of optimized Boron Nitrogen Atom no. Isotropic Anisotropic Atom no. Isotropic Anisotropic 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 36 39 40 41 44 45 46 50 52 53 54 a,b structure for B28N 28 cage (in ppm) 71 71 67 68 67 71 71 67 71 68 67 67 71 67 67 71 71 67 71 71 67 68 67 68 67 67 71 71 49 49 39 24 39 49 49 39 49 24 39 39 49 39 39 49 49 39 49 49 39 24 39 24 39 39 49 49

Firstly, the considered models were allowed to entirely relax during the geometrical optimization by the B3LYP exchange-functional method [48,49] and the 6-311++G (d, p) standard basis set. Then the quantum chemical calculations were performed on 14

18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 37 38 42 43 47 48 49 51 55 56 123 96 123 96 123 96 96 123 99 96 123 96 123 123 96 99 96 123 96 96 99 123 123 123 99 123 96 96 181 159 181 159 181 159 159 181 156 159 181 159 181 181 159 156 181 159 159 156 181 181 181 156 181 159 159 the

geometrical optimized models by the B3LYP method and the 6-311++G(d,p) standard basis set to evaluate 16

the total electronic energy, energy gap of HOMO-LUMO and, Nitrogen and Boron

NMR and NQR parameters, respectively (Tables 1- 1

7). a,b Table 5. NQR parameters of optimized structure of B₁₂N₁₂ cage Boron Atom no. c (MHZ) h Atom no. c (MHZ)

	1	2	3	4	9	12	14	16	17	20	22	24	1	2	3	4	5	6	7	8	17	20	21	24	27	28	29	32	3.22	3.22	3.22	3.22	3.22	3.22	3.22	3.22
Boron	3.13	3.13	3.27	3.27	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	3.13	0.11	0.11	
	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.067	0.067	0.00	0.00	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067	0.067		
	0.067	0.00	0.00	0.067	0.067	5	6	7	8	10	11	13	15	18	19	21	23	9	10	11	12	13	14	15	16	18	19	22	23	25	26	30	31	0.76	0.76	
	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76		
Nitrogen	0.74	0.74	0.74	0.74	0.98	0.74	0.98	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74	0.74		
	0.98	0.98	0.74	0.74	0.78	0.78	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.77	0.78	0.78	a,b Table 6.	NQR parameters of	optimized structure of B ₁₆ N ₁₆ cage	Atom no. c (MHZ)	h Atom no. c (MHZ)					

h 0. 65 0. 65 0. 65 0. 65 0. 002 0. 65 0. 003 0. 65 0. 65 0.
65 0. 64 0. 65 0. 001 0. 004 0. 65 0.

22

65 a See figures 3 and 6 for more details. b Compare the data with the results of [41–44] a a See figures 1 and 4 for more details. See figures 2 and 5 for more details. b Compare the data with the results of [42], [44]. 103 A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) Table 7. NQR parameters of optimized structure

for 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

21

[illegible]

methods reveals that GIAO is the method most commonly used to calculate absolute shieldings

1

[50].

Quantum chemical calculations do not directly yield experimentally measurable NMR and NQR parameters. The quantum calculations were adapted to reproduce reliable NMR and NQR properties

1

[51,52]. Table 8.

B3LYP/6-311++g(d,p)

43

calculated ionization potentials, IP, electronic affinities, EA, chemical potentials, μ , hardnesses, η , and electrophilicity values, ω (I,A), a (IP, EA, μ , η , and ω (I,A), in eV) for the

2

magic BN nanocages Nanocage IP EA μ η ω (I,A) B 12 N 12 9.59 -0.16 -4.71 9.75 1.14 B 16 N 16 9.12 0.20 -4.66 8.93 1.22 B 28 N 28 8.94 0.13 -4.54 8.82 1.17

Typically it is only necessary to report the three principal components (or eigenvalues) of the

3

boron and nitrogen atoms CSA (Chemical Shift Anisotropy) tensor (σ , σ , σ)

when discussing the magnitude σ_{11} , σ_{22} , σ_{33} of the shielding tensor. When the atoms CSA

3

tensor is described within the principal axis system (PAS) [53], the diagonal representation of the tensor is obtained. The

3

atoms

CSA tensor can also be described by two additional parameters; a) the isotropic value (or

3

trace), σ , of the shielding tensor iso which is defined as:

The most commonly used methods of calculating chemical shifts are the individual gauge for localized orbitals (IGLO) method, the localized orbital/local origin (LORG) method, and the gauge-independent or -invariant or -including atomic orbital (GIAO) method. Reviewing Chemical Abstracts (for works published between 1987 and 2001) for the mentioned

9

$$\sigma = 1/3(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad (1)$$

iso 11 22 33 b) the anisotropy ($\Delta\sigma$) of the tensor, given by

28

$$D\sigma = \sigma_{11} - 1/2(\sigma_{22} + \sigma_{33}) \quad (2)$$

33 11 22 a See figures 3 and 6

for more details. b Compare the data with

4

the results of [42], [44].

a See figures 1- 3 for more details.

4

A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 104 The

assignment or ordering of the principal components in the atoms CSA tensor depends on the convention used, but for this manuscript the principal components are defined using: $\sigma_1 \geq \sigma_2 \geq \sigma_3$

3

The NQR parameters are the nuclear quadrupole coupling constant c and the asymmetry parameter h . However, Eqs. 3 and 4 are used to relate the calculated EFG tensors to their associated experimentally measurable parameters:

1

$2c = eQq_{zz}/h$ (3) $h = |q_{xx} - q_{yy}|/|q_{zz}|$ (4) Here, c

is the interaction energy for the nuclear electric quadrupole moment eQ and the EFG tensors, whereas h is a measure of the deviation of the EFG tensors from cylindrical symmetry at the sites of the quadrupole nuclei. Quadrupole nuclei are those that have a nuclear spin angular momentum of greater than one-half ($I > 1/2$). The EFG tensor eigenvalues were calculated in the principal axis system (PAS) using the relation

1

$|q_{xx}| \geq |q_{yy}| \geq |q_{zz}|$. The

standard Q values reported by Pyykkö [54] 14 were employed

34

in Eq. 3: $Q(N) = 20.44$ mb and 11 $Q(B) = 40.59$ mb. Tables 5, 6 and 7 show the calculated NQR parameters for N and B nuclei in the three

1

magic BN fullerenes. The density functional theory

method utilized in the present study presumes the selection of isolated clusters for all of the actual calculations

1

and ignores

interactions among adjacent clusters. In this manner it is possible to obtain discrete clusters

1

for the geometry optimization and all of the calculations.

+ -

The energies, $E(M^+)$ and $E(M^-)$, of the ionic states of each cluster M were calculated at the B3LYP/ 6-311++g(d,p)

7

level using the optimized geometries of the neutral cages. The $IP = E(M^+) - E(M)$ and the $EA = E(M) - E(M^-)$ values determined by these DFT energies are the computed vertical ionization potentials and the vertical electron affinities from the bottom of the potential well of the neutral species, respectively [55]. The global electrophilicity index ω , which measures the stabilization in energy when the system acquires an additional electronic charge ΔN from the environment, has been given the following simple expression

2

[56]: $2\omega = \mu^2 / 2\eta$ (5)

in terms of the electronic chemical potential μ and the chemical hardness η . The natural way to approximate the μ and η in DFT is evaluating directly from the IP and EA energies: $\mu = -(IP + EA)/2$ (6) $\eta = IP - EA$

2

(7) The

electrophilicity index encompasses both, the propensity of the electrophile to acquire an additional 2 electronic charge driven by μ (the square of electronegativity) and the resistance of the system to exchange electronic charge with the environment described by η , simultaneously. A good electrophile is, in this sense, characterized by a high value of μ and a low value of η . 3. Results and discussion

2

and the HOMO–LUMO energy gap (in eV) of the

23

of magic BN fullerenes (Figures 1-3). As the table contents present

the total energy of the magic BN clusters increases with increase of the

39

size of the nanocages from B₁₂N₁₂ to B₂₈N₂₈ (Figures 1-3). Inspection of the energy gap of HOMO-LUMO (Table 1) indicates that the B₁₂N₁₂ (Figure 2) and B₁₆N₁₆ the BN cluster (Figure 3) nanocages have the smallest and the largest energy band gap respectively but in this case there is not a regular order with respect to cluster size like the total energy of clusters (Table 1). 3.1. NMR parameters Tables 2, 3 and 4 present the isotropic (σ) and iso anisotropic (D_s) nuclear magnetic shieldings of boron and nitrogen atoms calculated for fully optimized B₁₂N₁₂, B₁₆N₁₆ and B₂₈N₂₈ fullerenes (Figure 1-3), respectively.

Boron and nitrogen atoms adopt different roles in the magic fullborenes

1

due to lack

of electrons in valence shell of boron atoms and

25

the presence of

lone pair of electrons in the nitrogen atoms valence shell.

25

Nitrogen nuclei have greater isotropic and anisotropic chemical shielding than boron nuclei.

1

As table 2 presents the B₁₂N₁₂ fullborene just show one peak (64 ppm) for boron atoms and also one peak (107

ppm) for nitrogen atoms. In table 3 peak at ~66 -68 ppm is assigned to boron atoms, and peaks at

1

~ 93-94 ppm and ~ 130- 131

ppm reflect the chemical shieldings of nitrogen atoms in the

1

B N magic BN fullerene. The results 16 16

of our calculations, as shown in Table 4, also predict ~67–68 ppm and 71 ppm shielding of the signals from boron atoms and ~96–99 ppm and 123 ppm chemical shieldings from nitrogen atom signals in B N fullborene.

1

28 28 3.2.

NQR parameters The results from quantum chemical calculations of NQR parameters (c,h) for fully relaxed magic fullborenes are shown in tables 5, 6 and 7. Since there is no experimental NQR data for these BN fullerenes available in the literature, the tables do not reference any experimental data for the calculated results

1

but they reference some theoretical researches on related BN materials.

A quick look at the results from the calculations

1

(Tables 5, 6, 7)

reveals that the NQR parameters vary for the nuclei; therefore, the electrostatic

1

environments of these magic full- borenes

with different structures are not equivalent, although these differences are not very conspicuous. In the

1

table 5 NQR parameters of B N fullborene 12 12 (Fig. 1) are collected. As we can see the whole cluster has a uniform electrostatic environment due to the fact that all of boron atoms have the same c quantity (3.22 MHz) and so do the nitrogen atoms (0.76 MHz). The B N structure can be imagined 12 12 as six tetragons whose corners are chemically bonded together. The c parameters of B N (Table 6) and 16 16 B N (Table 7) do not present the trend. One can 28 28 imagine a B N cluster as six BN tetragons whose 16 16 corners bind together by boron or nitrogen atoms (Fig. 2). In the B N cluster the boron atoms (B3, 16 16 B4, B27, B28- see Fig. 5) and also the nitrogen atoms (N13, N15, N25, N26- see Fig. 5) which bind corners of three tetragons have different c values and their quadrupole coupling constants are the largest (3.27 MHz for the boron and 0.98 MHz for nitrogen atoms). Table 7 shows NQR parameters of B N fullborene and also this magic fullborene 28 28 does not have a uniform electrostatic environment in the whole cage. The 12 nitrogen

atoms which are located at the corners of the

37

6 tetragons (Fig. 6) have the smallest c values (0.36 MHz). Among the A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 106 boron atoms those borons which do not directly have chemical bonds with corners of a tetragon or included in a tetragon corners (B4, B10, B44, B46) show the smallest quadrupole coupling constants (2.94 MHz) (Table 7).

To the best of our knowledge there is no experimental data on NMR and NQR spectroscopic parameters

4

of magic BN fullerenes but

comparing the c values computed in this work with experimental nitrogen and boron NQR

1

parameters of some related BN material

verifies the c values calculated in this work for the clusters.

1

A.H.

Silver et al. reported the magnitude of the coupling

4

2 constant of boron atom $e Qq_{zz}/h=2.96\pm0.10$ [57] and M. Khusidman research group

in two studies find that the experimental value is 2.44 [58,59] and the

4

3.00 ± 0.10 value reported by M. Fanciulli research crew [60]. Also c

$=2.9$ MHz [61] and more precise value of $2.934\pm$

4

0.004 MHz have been obtained by other researchers [62]. A quadrupole coupling constant of $2.936\pm$

4

0.020 were obtained by G. Jeschke et al.

4

in cubic and hexagonal boron nitride for boron

8

atoms[63]. Considering the fact that BN nanocages have structures different from the mentioned BN compounds,

the theoretical values of this study

4

(Tables 5, 6 and 7)

are in good agreement with the 14 experimental data. The

33

N NQR experimental value reported by Jeschke and his co-workers was 140 ± 10 kHz [63]. Palmer et al. in their theoretical study found values between 0.753 and 1.328 MHz 14 for N quadrupole coupling constants [64]. The

disagreement between experimental and theoretical 14 values for N in the presence of a better agreement 11 for B (theoretical values between 2.773 and 3.604 MHz), suggests difficulties in describing correctly the distribution of the nitrogen lone pair in the theoretical calculations

8

[63]. Bagheri et al [65] performed a DFT based calculation for (6,0) single-walled BNNT in three forms of H-capped, N-end and B-end tubes. They calculated the EFG tensors using

B3LYP level of theory with 6-311++G**, 6-31++G**

38

and CC-pVTZ standard basis sets. Their result showed four equivalent electrostatic layers in the tube length. Comparing our NQR quadrupole coupling constants with the mentioned researches results reveals that the B atoms χ are more consistent in the two researches than N atoms regarding the structural difference between BN nanocages and BNNTs and, the B3LYP with

6-31+G** standard basis set in the

20

Baghrei research group presents the best consistency with our results. In the case of N atoms the differences are more conspicuous than that of B atoms and as we mentioned earlier this is due to nitrogen lone pairs and the

difficulties in describing correctly the distribution of the nitrogen lone pair in the calculations. theoretical

8

Figure 4. 2D views of B N magic BN fullerene 12 12 Figure 5. 2D viewsof B N magic BN fullerene 16 16 Figure 6. 2D views of BN magic BN fullerene 28 28 107 A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 4.

Evaluation of the electrophilicity indexes from the IPs and EAs, ω (I,A), With the IP and

2

EA values calculated in the com- putational methods Section,

we have computed the electrophilicity indexes, ω (I,A).

2

The corresponding values are collected

in Table 8. It is observed that irrespective of the increase in nanocage size, electrophilicity does not change

15

significantly. For these BN nanocages,

it is observed that even though the size of the nanocage increases, it does not affect the chemical potential of the

15

cluster. Evaluating the values of hardnesses in table 8 shows that B N has the largest hardnesses. It is meant 12 12 that B N has the largest

resistance of the chemical 12 12 potential to change in the number of electrons

18

among magic BN fullerenes. 5.

Concluding remarks The goal of this study was, for the first time, to calculate the NMR and NQR parameters at the locations of N and B nuclei and the

1

electrophilicity index, ω , in the three stable structures of magic fullborenes:

B N , B N and B N

24

(Fig.s 1-3). 12 12 16 16 28 28

Optimization of geometries and NMR and NQR calculations of the considered structures were performed.

1

All of these magic fullborenes cages have just squares and hexagons, and the

1

number of tetragons is different in the three fullborenes. B N cluster hassix tetragons and eight hexagons 12 12 (Fig. 1). The B N structure consists of six tetragons 16 16 and twelve hexagons (Fig. 2) while there are six tetragons and twenty four hexagons in B N 28 28 structure

(Fig. 3). The energies of these three

1

BN fullerenes are different

(Table 1). The most stable structure is the

1

B Nfullborene (Fig. 3) with the 28 28 . maximum energy band gap between HOMO and LUMO (Table 1). The magic fullborenes with energy gap varying from 6.25 to 6.80 eV are wide band gap clusters. The

calculated chemical shieldings (s) indicated iso that the N nuclei in B N fullborene show peak at

1

12 12 107 ppm, and also one peak for B nuclei close to 64 ppm (Table 2, Fig. 4). The components at ~ 93-94 ppm and ~ 130-131

ppm correspond to N nuclei and at ~66 -68 ppm to B nuclei in the B N model

1

16 16 (Table 3, Fig. 5),

so this model shows two peaks for N and one peak for B nuclei, respectively. The

1

B N cluster shows two peaks at ~96–99 ppm and 28 28

123 ppm which are attributed to N nuclei and two peaks at ~67–68 ppm

1

and 71

ppm which reflect the chemical shielding of B nuclei

1

(Table 4, Fig. 6). As it can be seen,

NMR quantum calculations are a useful tool for studying the structural features of three magic BN fullerenes, since the positions of the NMR signals in each model are well reflected in the NMR chemical shieldings. The predicted NMR parameters may aid experimentalists in identifying the structure of magic fullborenes. In addition, we can see that the nuclear magnetic shielding tensors of N nuclei display substantial sensitivity to structural changes, while B nuclei do not

1

show this feature. The calculated NQR parameters

(Tables 5, 6 and 7)

revealed that the electrostatic environments of the three magic clusters are as different as their structures. The c values of the B nuclei in all the cages do not show tangible changes, whereas the c values of the N nuclei do show more variations. As the NQR calculations show, the electrostatic environment of the

1

B N is homogeneous throughout the cluster $12\ 12$ (Table 5), but the B N and B N cages do not $16\ 16\ 28\ 28$ exhibit this characteristic (Tables 6, 7). The c values A. Boshra et al. / Journal of Nanostructure in Chemistry 2 (2) (2011) 108

of the B nuclei in all of the cages are greater than of

1

those of the N nuclei. The calculated NQR parameters will play a key role when studying the interactions of atoms and molecules with the clusters, which are important in catalysis as well as in the development of cluster-based materials.

1

The electro- philicity indexes, $\omega(I,A)$ which have computed via the IP and EA values (Table 8) presents the largest hardness for B N nanocage. Due to thisfact, B N $12\ 12\ 12\ 12$ has the largest

resistance of the chemical potential to change in the number of electrons

18

among magic BN fullerenes. The results show that there is no considerable change in electrophilicity index of these BN clusters with the change of their sizes. References [1] S. Iijima, Nature 354 (1991) 56. [2] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.E. Smalley, Nature 318 (1985) 162. [3] T. Oku, T. Hirano, M. Kuno, T. Kusunose, K. Niihara, K. Suganuma, Mater. Sci. Eng. B 74 (2000) 206. [4] T. Oku, A. Nishiwaki, I. Narita, M. Gonda, Chem. Phys. Lett. 380(2003) 620. [5] R. Ma, Y. Bando, T. Sato, L. Bourgeois, Diamond Relat. Mater. 11(2002) 1397. [6] C. Tang, Y. Bando, T. Sato, Chem. Phys. Lett. 362 (2002) 185. [7] B. G. Demczyk, J. Cumings, A. Zettl, R. O. Ritchie, Appl. Phys. Lett., 78(2001) 2772. [8]

T. Hirano, T. Oku, K. Suganuma, *Diamond Relat. Mater.* 9(2002) 625. [9] O. Ste'phan, Y. Bando, A. Loiseau, F. Willaime, N. Shramchenko, T. Tamiya, T. Sato, *Appl. Phys. A.* 67(1998) 107. [10] A. Loiseau, F. Willaime, N. Demoncy, G. Hug, H. Pascard, *Phys. Rev. Lett.* 76(1996) 4737. [11] N. G. Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, S. G. Louie, A. Zettl, *Science*, 269(1995)966. [12] S. S. Alexandre, M. S. C. Mazzoni, H. Chacham, *Appl. Phys. Lett.*, 75(1999) 61. [13] S. S. Alexandre, H. Chacham, R. W. Nunes, *Phys. Rev. B*, 63(2001) 0454021. [14] G. Seifert, R. W. Fowler, D. Mitchell, D. Porezag, T. Frauenheim, *Chem. Phys. Lett.*, 268(1997) 352. [15] P. Gleize, M. C. Schouler, P. Gadelle, et al., *J. Mater. Sci.*, 29 NQR 1575. [16] N. G. Chopra, R. J. Luyken, K. Cherrey, et al., *Science*, 269(1995) 966. [17] A. Loiseau, F. Willaime, N. Demoncy, et al., *Phys. Rev. Lett.*, 76(1996) 4737. [18] A. Zettl, *Adv. Mater.*, 8(1996)443. [19] I. Narita and T. Oku, *Diamond Relat. Mater.*, 12 (2003)1146. [20] F. L. Deepak, C. P. Vinod, K. Mukhopadhyay, et al., *Chem. Phys. Lett.*, 353(2002) 345. [21] N. G. Chopra, R. J. Luyken, K. Cherrey, et al., *Science*, 269(1995) 966. [22] F. Jensen and H. Toftlund, *Chem. Phys. Lett.*, 201 (1993) 89. [23] I. Silaghi-Dumitrescu, F. Lara-Ochoa, P. Bishof, et al., *J. Mol. Struct. (Theochem)*, 367(1996) 47. [24] I. V. Stankevich, A. L. Chistyakov, and E. G. Galperin, *Izv. Akad. Nauk, Ser. Khim.*, 10(1993)1712. [25] I. V. Stankevich, A. L. Chistyakov, E. G. Galperin, et al., *Zh. Strukt. Khim.*, 36(1995)976. [26] H. -Sh. Wu, X. -Y. Cui, X. -F. Qin, H. Jiao, *J. Mol. Struct.:THEOCHEM*, 714(2005)153. [27] S. S. Alexandre, M. S. Mazzoni, and H. Chacham, *Appl. Phys. Lett.*, 75(1999) 61. [28] V. V. Pokropivny, V. V. Skorokhod, A. V. Kurdyumov, et al., *J. Solid State Chem.*, 154(2000)214. [29] P. W. Fowler, K. M. Rogers, G. Seifert, et al., *Chem. Phys. Lett.*, 299(1999)359. [30] M. Mileev, S. Kuzmin, V. Parfenyuk, *J. Struct Chem.* 47 (2006) 1016. [31] D. L. Strout, *Chem. Phys. Lett.* 383 (2004) 95. 109 A. Boshra et al. / *Journal of Nanostructure in Chemistry* 2 (2) (2011) [32] V. Pokropivny, L. I. Ovsyannikova, S. V. Kovrigin, *Phys. Sol. State*, 49 (2007) 2335. [33] T. Oku, A. Nishiwaki, I. Narita, *Sci. Tech. Adv. Mater.*, 5 (2004) 635. [34] A. N. Enyashin, A. L. Ivanovskiĭ, *Phys. Sol. State*, 50 (2007) 390. [35] J. M. Matxain, L. A. Eriksson, J. Poater, E. Matito, M. Solà, *J. Phys. Chem. C* 111 (2007) 13354. [36] D. M. Sheichenkov, A. V. Pokropivny, V. V. Pokropivny, *Semicond. Phys. Quant. Electron Optoelectron* 3(4) (2000)545. [37] Y.-Z. Lan, W. -D. Cheng, D. -S. Wu, X. -D. Li, H. Zhang, Y. -J. Gong, J. Shen, F. -F. Li, *J. Mol. Struct. (Theochem)*, 730(2005)9. [38] S. A. Shevlin, Z. X. Guo, H. J. van Dam, P. Sherwood, C. R. A. Catlow, A. A. Sokol, S. M. Woodley, *Phys. Chem. Chem Phys.*, 10 (2008) 1944. [39] J. K. Jung, K. -S. Ryu, Y. -I. Kim, C. Tang, *Sol. State Comm.* 130 (2004) 45. [40] J.N. Latosin'ska, M. Latosin'ska, J. Koput, *J. Mol. Struct.* 648 (2003) 9. [41] A. Boshra, M. M. Dehshiri, A. Seif, R. Jafari, *J. Mol. Struct.: THEOCHEM*, 906 (2009) 63. [42] Ahmad Seif, Asadollah Boshra, Majid Seif, *J. Mol. Struct.: THEOCHEM*, 895 (2009) 82. [43] A. Seif, A. Boshra, *J. of Mol. Struct.: THEOCHEM*, 895 (2009) 96. [44] G. M. Rouzbehani, A. Boshra, A. Seif, *Monatsh Chem* 140 (2009)255. [45] T. P. Das, E. L. Han, *Nuclear quadrupole resonance spectroscopy*. Academic press, New York (1958). [46] W. C. Bailey, *Chem. Phys.* 252(2000) 257. [47] M. J. Frisch, G.W. Trucks, H. B. Schlegel, G.E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J.A. Montgomery Jr., R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, A.G. Baboul, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C.Y. Peng, A.

Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head- Gordon, E.S. Replogle, J.A. Pople, Gaussian 98, Revision A.7, Gaussian, Inc., Pittsburgh, PA, 1998. [48] A.D. Becke, J. Chem. Phys. 98 (1993) 5648. [49] C. Lee , W. Yang , R. G. Parr , Phys. Rev. B 37 (1988) 785. [50] I. Alkorta, J. Elguero, Struct. Chem., 14(4) (2003) 337. [51] M. Schindler, W. Kutzelnigg, J. Am. Chem. Soc., 105(1983) 1360. [52] U. Fleischer, W. Kutzelnigg, A. Bleiber, J. Sauer, J. Am. Chem. Soc. 115(1993) 7833. [53] J. Mason, Solid State Nucl. Magn. Reson., 2(1993)285. [54] P. Pyykkö, Mol. Phys., 99(2001) 1617. [55] C.-G. Zhan, J.A. Nichols, D.A. Dixon, J. Phys. Chem. A 107 (2003) 4184. [56] R.G. Parr, L. von Szentpaly, S. Liu, J. Am. Chem. Soc. 121 (1999)1922. [57] A.H. Silver, P.J. Bray, J. Chem. Phys.32(1960)288. [58] M. Khusidman, V. Neshpor, Zh. Strukt. Khim., 12 (1971)1094. [59] M. Khusidman, V. Neshpor, J. Struct. Chem.,12 (1971)1008. [60] M. Fanciulli, M. Corti, Phys. Rev. B: Condens. Matter., 52(1995)11872. [61] P. S. Marchetti, D. Kwon, W. R. Schmidt , L.V. Interrante, G.E. Maciel, Chem. Mater., 3(1991) 482. [62] C. Connor, J. Chang, A. Pines, Rev. Sci. Instr., 61 (1990)1059. [63] G. Jeschke, W. Hoffbauer, M. Jansen, Solid State Nucl Magn Reson., 12(1998)1. [64] M.H. Palmer, J.A. Blair-Fish, Z. Naturforsch., 49a (1994)137. [65] Z. Bagheri , M. Mirzaei, N. L. Hadipour, M. R. Abolhassani, J. Comput. Theor. Nanos., 5(2008).