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The Nitrogen atom effect on structural and magnetic properties of Fullerene C_{20}:A DFT study

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ABSTRACT: The fullerene structures of C_{20cage} and bowl,$C_{20}H_{10}$ and their N-doped structures as C_{20cage} NH,C_{20bowl} NH, $C_{20}H_{10}NH$, $C_{20}H_{10}N$ and their isomers are optimized using the MPW1PW91/6-31G level of the theory. Magnetic shielding tensors of ^{14}N and ^{13}C atoms are calculated by the same level of the theory. Results show that doping an N atom on fullerenes affects differently on the chemical shielding of C atoms which are connected to the N atom to be distinguishable experimentally. The maximum chemical shielding of N and N-connected C atoms were shown in the isomer of $C_{20}H_{10}NH$. It seems that this structure with maximum bond length of C-N is the suitable molecule for additional reactions.

Keywords: *Bowl; C_{20}; Cage; DFT; Nano Fullerene; NMR*

INTRODUCTION

Carbon has been found in several forms comprising amorphous, graphite and diamond. Fullerenes are the fourth form of solid carbon. Increasing attention has been attracted variety of fullerene structures since the discovery of C_{60} (Kroto, *et al.*, 1985). These structures can provide different doping possibilities including-substitutional doping, endohedral doping and exohedral doping (Türker, 2002, Türker, 2003, Lee, 1995, Lee, 2011, Tang, et al., 2012, Wang and Zhang, 2011). The smallest available fullerene is C_{20}. (Prinzbach, *et al.*, 2000) indicated experimental evidence for the existence of three different isomers, namely cage, bowl and ring. The smallest possible cage fullerene, C_{20cage}, is composed of solely by pentagons and is of extreme curvature and large reactivity. In $C_{20\ bowl}$, one central pentagonthat is surrounded by five hexagons is seen. C_{20ring} structure with the highest symmetry, D10h, is found. Although there is general agreement that the cage, ringand bowl isomers are three main candidates of the ground state structure(Saito and Miyamoto, 2001) the scientist disagree on the fact that which of these is the most stable. (Sokolova, *et al.*, 2000) showed that different quantum mechanical methods calculated different total energy for this C_{20} isomer, respectively. DFT/LDA calculations indicated the cage as the lowest energy geometry (Grossman, *et al.*, 1995) while DFT with gradient x-functional corrected function predicted the ring to be the most stable one. However, (Grossman, 2002) using a high-level MP2/TZV2df calculation found the cage and bowl to be of the lowest energy and to be al-

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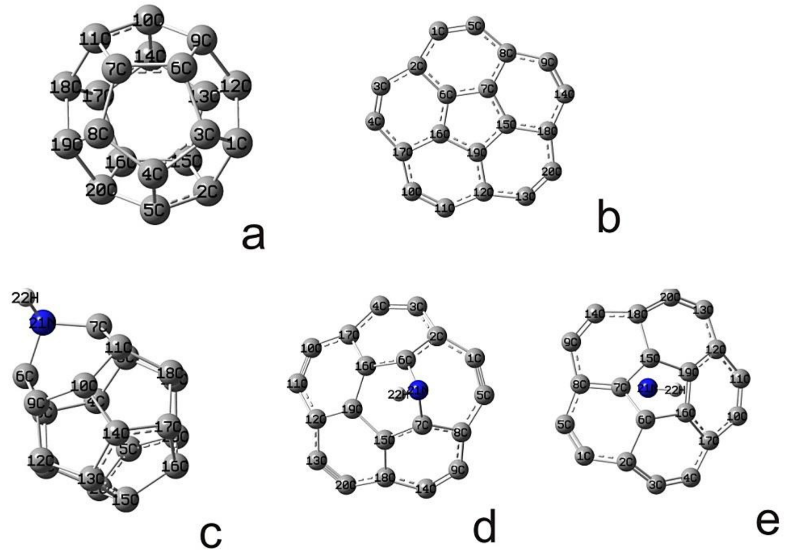

Fig.1.The optimized structures of two isomers of C_{20} and their N-doped structures, (a:C_{20cage} b: C_{20bowl} c: C_{20cage} NH d: C_{20bowl} NH1 e: C_{20bowl} NH2).

most isoenergetic isomers. Also (Brabec, *et al.*,1992) showed that the bowl is the most stable configuration Finally, The new benchmark study of (Jin, *et al.*,2015) indicated that the bowl is the most stable at 0 K. Since corannuleneis relatively easy to synthesize and has both concave and convex surfaces to react with the nitrogen, we can compare it with fullerene. Severals to investigate corannulene-based materials were studied by (Banerjee, *et al.*,2011, and Zhang, *et al.*,2012).

Due to the high sensivity of the NMR signals to the electronic density at the sites of magnetic nuclei such as ^{14}N and ^{13}CNMR has been approved as apowerful tool for investigating the structural properties of various materials. Despite the theoretical and experimental studies, spectroscopic data are used in order to determine the actual structure of fullerene produced in experiments. Owing to the complexity in Nano cages, the electrostatic environment around the nucleus is not exploring directly by practical spectroscopy data. Nevertheless, quantum calculations play an important role in evaluating the NMR parameters of nanocages. Many attempts to discriminate different fullerene isomers have been reported (Galli, *et al.*, 1998, Jones and Seifert, 1998). These calculated results have been successfully fitted to the experimental results within a few ppm are approved due to the fact that NMR technique is as much accurate for the fullerenes as for many others molecules and atomic clusters (Fowler, *et al.*, 1991, Saunders, *et al.*, 1996). The calculations of nuclear magnetic resonance (NMR) parameters using ab initio techniques are appropriated to quickly evaluated and correlated the magnitude of the chemical shielding (CS) tensor with variations in bond angles, bond length, the nearest neighbor interactions and electrostatic environment around magnetic nuclei like ^{13}C (Ditchfield, *et al.*, 1998) and ^{17}O (Mason, 1993). Here, we report relative stability of some isomers and the calculated chemical shielding in N-doped fullerenes C_{20} in order to compare the N atom effect on chemical shielding of neighbor atoms which were connected to the N atom.

RESULTS AND DISCUSSION

All density functional theory (DFT) calculations were performed using Gaussian 98 program package (Frisch, *et al.*,1998).The optimized geometry and calculated nuclear magnetic resonance (NMR) parameters were studied at MPW1PW91/6-31G levelof the theory (Adamoand Barone, 1998). The ^{13}C and ^{14}N chemical shielding tensors at the sites were calculated at the same level based on the gage independent atomic orbital (GIAO) approach (Adamo and Barone,1998).

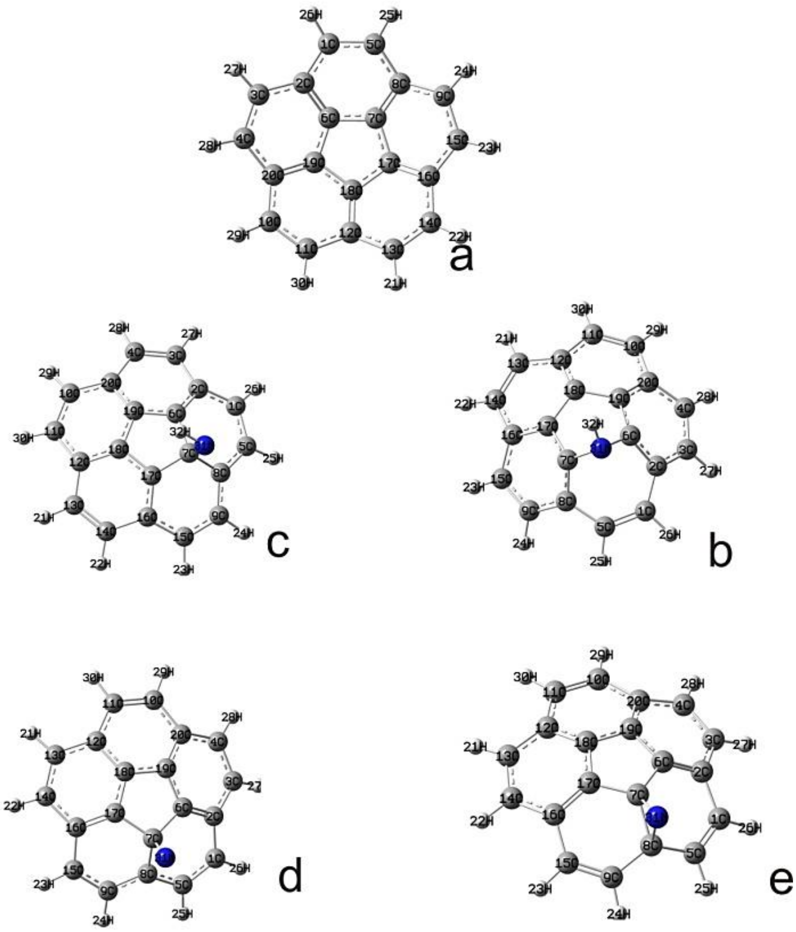

Fig.2.The optimized structures of $C_{20}H_{10}$ and its NH-doped and N-doped structures a: $C_{20}H_{10}$, b: $C_{20}H_{10}NH1$, c: $C_{20}H_{10}NH2$, d: $C_{20}H_{10}N1$, e: $C_{20}H_{10}N2$

RESULTS AND DISCUSSION

Geometry optimization

The optimized structures of $C_{20cage,bowl}$ and $C_{20}H_{10}$ have been shown in (Figs. 1-2) respectively. In order to obtain the most stable N-doped structure, an N atom or an NH group were doped on pentagon in such a way that N atom is connected to C_6 and C_7 atoms. The op-

Table 1. Optimized equilibrium geometries of N-doped structures at the MPW1PW91/6-31G level of the theory

structures	Bond length (Å)	Bond angle (◦)	Dihedral Angle (◦)
C_{20cage}	C_1-C_2:1.45,C_1-C_3:1.45,C_1-C_{12}:1.44	------------	----------
C_{20cage} NH	C_1-C_2 :1.47, C_1-C_3:1.48, C_1-C_{12}:1.48,C_6-N:1.42;C_7-N:1.42,	$<C_6NC_7$:103.972	----------
C_{20bowl}	C_6- C_7:1.41, C_7-C_{15}:1.41,C_7-C_8:1.41	------------	180.00,179.99
C_{20bowl} NH1	C_7-C_{15}:1.43, C_7-C_8:1.41,C_6-N:1.420; C_7-N:1.42	$<C_6NC_7$:100.705	140.97,128.59,90.56
C_{20bowl} NH2	C_6- C_7:1.48, C_7-C_{15}:1.48, C_7-C_8:1.36,C_6-N:1.62,C_{15}-N:1.6119	$<C_6NC_{15}$:78.705	160.20,123.05,158.87
$C_{20}H_{10}$	C_6- C_7:1.46, C_6- C_2:1.43, C_2-C_1:1.50	------------	153.29
$C_{20}H_{10}$ NH 1	C_1-C_2 :1.46, C_6- C_2:1.38,C_6-N:1.426; C_7-N:1.426	$<C_6NC_7$:96.647	165.59, 87.91,126.01
$C_{20}H_{10}$ NH2	C_6- C_7:1.46, C_6- C_2:1.38,C_7-C_{17} :1.46,C_6-N:2.42;,C_6-C_{19}:1.39, C_{17}-N: 2.42	$<C_6NC_{17}$:56.57	148.06,152.81, 100.09
$C_{20}H_{10}$ N1	C_6- C_7:1.50, C_7-C_{17}:1.50 ,C_6-C_{19}:1.39,C_6-N:2.34; C_7-N:1.47; C_{17}-N:2.49	$<C_6NC_7$:33.54; $<C_6NC_{17}$:55.72	131.97,163.35, 145.55
$C_{20}H_{10}$ N2	C_6- C_7:1.46, C_7-C_8 :1.52, C_6-C_{19}:1.40,C_7-N:1.47; C_8-N:1.52	$<C_8NC_7$:61.049	141.63, 144.92, 160.66

Table 2.Total energy (a.u), relative energy (eV) and the calculated $^{13}C_6$ atom NMR parameters (in ppm) for fullerene C20 and N-doped structures.

Structure	C6								
	CSI	CSA	σ_{11}	σ_{22}	σ_{33}	h	E(a.u)	δ	E (eV)
C_{20cage}	44.852	-160.7639	-62.3239	45.7454	151.1345	0.983328342	-761.0698	154.638	0.00153
C_{20cage} NH	-35.319	172.75985	-165.149	59.1921	119.7814	1.446425025	-816.43046	234.8	0.0000
C_{20bowl}	50.4206	111.57505	-7.1676	33.6253	124.8039	0.548414765	-761.10713	149.069	0.0000
C_{20bowl} NH1	59.5129	155.26425	-38.1398	53.6561	163.0224	0.886835508	-816.37684	139.87	0.00233
$C_{20\ bowl}$ NH2	88.3162	64.79985	53.7117	79.7208	131.5161	0.602063894	-816.20002	111.18	0.01
$C_{20}H_{10}$	66.8266	170.9668	-12.3499	32.0251	180.8044	0.389330203	-767.81043	132.663	------
$C_{20}H_{10}$ NH1	64.3062	149.2531	-34.1054	63.2158	163.8083	0.97808187	-823.06270	135.19	0.000
$C_{20}H_{10}$ NH 2	89.9982	534.72205	-150.201	-26.2843	446.4796	0.34760944	-822.97029	109.5	0.00401
$C_{20}H_{10}$ N1	51.0367	172.8712	-20.5182	7.3442	166.2842	0.241761426	-822.37739	148.46	0.00096
$C_{20}H_{10}$ N2	62.6088	162.95695	-17.1237	33.7034	171.2468	0.467857472	-822.399477	136.89	0.0000
$Si(CH_3)_4$	199.49	7.2	197.07	197.1	204.3	-	-449.082259	-	-

CSI: Chemical shielding isotropy (in ppm); CSA: Chemical shielding anisotropy (in ppm); σ_{11}, σ_{22} and σ_{33} are the principal axis values of σ (in ppm);η: Asymmetry parameter;δ: Chemical shift with respect to TMS.

timized total energies and relative stability of parent structures and their doped-structuresat 298.14 K have been shown in Table 1. The calculated results (Table 1) showed that C_{20bowl} was more stable than C_{20cage} by 0.0015 eV while C_{20cage} NH was more stable than $C_{20\ bowl}$ NH1 or 2 isomers by 0.0023-0.0100eV. The 20 carbon atoms in C_{20bowl} structure arein the same plane butin NH-dopedstructure are not (Table 1). In doped structures of $C_{20}H_{10}$, $C_{20}H_{10}$ NH1 is more stable than $C_{20}H_{10}$ NH2 by 0.00401 eV and $C_{20}H_{10}$ N2 is more stable than $C_{20}H_{10}$ N1 by 0.00096eV. It confirms that the bowl and cage are almost isoenergeticisomers (Grimme, and Mück-Lichtenfeld, 2002). The C-C bond lengths of C_{20bowl} are smaller than ones of cage while in NH-doped structures the smallest C-C bond length is seen in C_{20cage} NH.

^{13}C and ^{14}N NMR parameters

The evaluated NMR parameters at the sites of C and N nuclei were presented in Tables 1-4. The calculated chemical shielding (CS) tensors inprincipal axes system (PAS) ($\sigma_{33}>\sigma_{22}>\sigma_{11}$) have been converted to measurable NMR parameters chemical shielding isotropic (CSI), chemical shielding anisotropy (CSA) and asymmetry parameter ofthe chemical shielding (η), using the following equations (Mason,1993):

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

$$\text{when} \, |\sigma_{11} - \sigma_{iso}| \le |\sigma_{22} - \sigma_{iso}| \qquad (1)$$

$$\Delta\sigma = \sigma_{22} - \frac{\sigma_{22} + \sigma_{11}}{2} \qquad (2)$$

$$\eta = \frac{\sigma_{22} - \sigma_{11}}{\sigma} \qquad (3)$$

Table 3.The calculated ^{13}C7 atom NMR parameters(in ppm) for N-doped structures

Structure	C7						
	CSI	CSA	σ_{11}	σ_{22}	σ_{33}	h	δ
C_{20cage}	45.1611	-160.8722	-62.087	46.3908	151.1796	0.977069058	154.329
C_{20}cage NH	-35.3946	232.71975	-165.221	-60.7152	119.7519	0.67359109	234.88
C_{20bowl}	50.4202	111.47315	-7.0593	33.5844	124.7357	0.546907442	149.069
C_{20bowl} NH 1	59.5055	155.2798	-38.1612	53.6524	163.0254	0.886917395	139.99
C_{20bowl} NH 2	78.174	559.6812	-206.783	-9.9903	451.2948	0.527422218	121.32
$C_{20}H_{10}$	66.8537	170.832	-12.2346	32.054	180.7417	0.388878547	132.636
$C_{20}H_{10}$ NH1	64.3062	149.2531	-34.1054	63.2158	163.8083	0.97808187	135.19
$C_{20}H_{10}$ NH2	155.2037	163.2954	80.3095	121.2343	264.0673	0.375927307	44.29
$C_{20}H_{10}$ N 1	117.4143	70.33815	90.452	97.4845	164.3064	0.149971957	82.08
$C_{20}H_{10}$ N 2	122.845	-71.8746	74.9286	125.3105	168.2959	0.89709160	76.65
$Si(CH_3)_4$	199.49	7.2	197.07	197.1	204.3	-	-

CSI: Chemical shielding isotropy (in ppm); CSA: Chemical shielding an isotropy (in ppm); σ_{11}, σ_{22} and σ_{33} are the principal axis values of σ (in ppm); η: Asymmetry parameter;δ: Chemical shift with respect to TMS.

Table 4.The calculated $^{13}C_8$ atom NMR parameters (in ppm) for fulleneneC20

Structure	C8						
	CSI	CSA	σ_{11}	σ_{22}	σ_{33}	h	δ
$C_{20}H_{10}$ $C_{20}H_{10}$	71.7314	189.9299	-0.8301	17.6729	198.3513	0.146130269	127.7586
$C_{20}H_{10}$ N2	131.8935	-86.6069	74.1556	139.1373	182.3877	0.749081626	67.5965
$Si(CH_3)_4$	199.49	7.2	197.07	197.1	204.3	-	-

CSI: Chemical shielding isotropy (in ppm); CSA: Chemical shielding an isotropy (in ppm);σ_{11}, σ_{22} and σ_{33} are the principal axis values of σ (in ppm); η: Asymmetry parameter;δ: Chemical shift with respect to TMS.

Table 5. Energy (kcal/mol) and the calculated ^{14}N NMR parameter (in ppm) for N-doped structures

Structure	**N**							
	CSI	**CSA**	$\boldsymbol{\sigma_{11}}$	$\boldsymbol{\sigma_{22}}$	$\boldsymbol{\sigma_{33}}$	η	**E(a.u)**	δ
C_{20cage} NH	153.0474	**-196.0381**	22.3553	215.7644	221.0224	**0.040231965**	-816.43046	90.3102
C_{20bowl}NH 1	165.9433	**-96.2069**	101.8054	188.3762	207.6484	**0.30048068**	-816.37684	77.4143
C_{20bowl}NH 2	-264.74	**-1428.095**	-1216.8	61.9787	360.6055	**0.313662659**	-816.20002	508.0976
$C_{20}H_{10}$NH1	166.5964	**-65.8968**	122.6652	179.2596	197.8644	**0.423498561**	-823.06270	76.7612
$C_{20}H_{10}$NH2	1643.485	6669.64	-1172.62	13.1631	6089.9113	0.266682368	-822.97029	-1400.1274
$C_{20}H_{10}$ N1	-157.476	610.8286	-494.363	-227.807	249.7436	0.654574896	-822.37739	400.8336
$C_{20}H_{10}$ N2	-174.323	754.30925	-448.631	-402.889	328.5494	0.090960776	-822.39948	417.6806
NH3	243.3576	28.6854	205.2545	262.3371	262.4811	-	-174.37599	-

CSI: chemical shielding isotropy (in ppm); CSA: chemical shielding an isotropy (in ppm); σ_{11}, σ_{22} and σ_{33} are The principal axis values of σ (in ppm); η: asymmetry parameter; δ: chemical shift with respect to NH_3

$$\sigma = \sigma_{33} - \sigma_{iso}$$
$$\text{when } |\sigma_{11} - \sigma_{iso}| \geq |\sigma_{22} - \sigma_{iso}| \qquad (4)$$

$$\Delta\sigma = \sigma_{11} - \frac{\sigma_{22} + \sigma_{33}}{2} \qquad (5)$$

$$\eta = \frac{\sigma_{22} - \sigma_{33}}{\sigma} \qquad (6)$$

$$\sigma = \sigma_{11} - \sigma_{iso} \qquad (7)$$

In the Tables 2-5, the numbers of Δσ and η that are not bold follow the rule of $|\sigma_{11}-\sigma_{iso}|<|\sigma_{33}-\sigma_{iso}|$ and other numbers that are bold (underlining) follow the rule of $|\sigma_{11}-\sigma_{iso}|>|\sigma_{33}-\sigma_{iso}|$. After doping NH on C_{20cage} structure, σ_{iso} of C_6 and C_7 was decreased from 44.852 and 45.1611 ppm to -35.319 and -35.3946 ppm, consequently. But after doping NH on $C_{20\ bowl}$ structures in C_{20bowl} NH_2 ,σ_{iso} of C_6 and C_7 increased from 50.4206 and 50.4202 ppm to 88.3162 and 78.174 ppm, respectively. However, after doping NH on C_{20bowl} structurein C_{20bowl} NH1, σ_{iso} of C_6 was decreased from 50.4202 ppm to-35.319, but σ_{iso} of C_7 increased from 50.4202 to 59.50559 ppm, consequently. While after doping NH on $C_{20}H_{10}$ in form of $C_{20}H_{10}$NH1, σisoof C_6 and C_7 was decreased from 66.8537 ppm to 64.3062 ppm, butin $C_{20}H_{10}$NH2, σisoof C_6 and C_7 increased from 66.8537 ppm to 89.9982 and 155.2037 ppm, respectively. Nevertheless, after doping N on $C_{20}H_{10}$ structure in $C_{20}H_{10}$N1 and $C_{20}H_{10}$N2 σ_{iso} of C6 was decreased from 66.8266 ppm to 51.0367 and 62.6088 ppm, respectively. In contrast, σ_{iso} of C_7 increased from 66.8537 ppm to 117.4143 and 122.845 ppm, respectively. There are maximum chemical shielding of C_6, C_7 and Natoms (Tables 2-5), and maximum bonding length of C-N in $C_{20}H_{10}$NH2 structure (Table 5). On the contrary, there is the minimum chemical shielding of C6 and C_7 atomsin C_{20cage} NH structure.The $C_{20}H_{10}$ NH_2 structure with maximum chemical shielding of C_6, C_7 and N atoms seems to be suitable for additional reactions. The ^{13}C and ^{14}N chemical shift ($\delta=\sigma_{iso}^{(TMS\ or\ NH3)}-\sigma_{iso}^{sample}$) are calculated with respect to TMS and NH3at MPW1PW91/6-31G level of the theory using the GIAO method also listed in tables (2-5). The $^{13}C_6$ chemical shift for C_{20cage} and $C_{20\ bowl}$ is 154 and 149 respectively. And it is obvious that variety in ^{14}N chemical shift for NH-doped structures show that their electrostatic environmentare sufficiently different chemically to be distinguishable experimentally.

CONCLUSIONS

The geometric structures and magnetic shielding tensors of the C_{20cage} andbowl ,$C_{20}H_{10}$ and their different N-doped structures for C_6, C_7 and N atomsare calculated using density functional theory in order to determine more stablestructures that can be of maximum chemical shielding. Chemical shift of ^{13}C and ^{14}N atoms was calculated with respect to TMS and NH_3 as for comparison, respectively. Results showed that maximum chemical shielding of C_6, C_7 and N atoms, andmaximum bond length of C-N are in $C_{20}H_{10}NH_2$, however, there isa minimum chemical shielding of C_6 and C_7 atoms in C_{20cage} NH, buta minimum chemical shielding of anN atom in the form of C_{20bowl} NH_2. So, $C_{20}H_{10}NH_2$ with maximum chemical shielding could be more suitable to contributein additional reactions. Finally, the NMR chemical shift of ^{13}C and ^{14}N show that they are sufficiently different chemically to be distinguishable experimentally.

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REFERENECES

Kroto, H.W.H.J.R.; O'Brien, S.C.; Curl, R.F.; Smalley, U.S.; (1985).C60-Buck minster fullerene. Nature, 318: 6042.

Türker, L.; (2002). Substitutional doping of B, Al and N in C60 structure. Mol. Struct. THEOCHEM, 593:1-3.

Türker, L.; (2003). Endohedral and substitutional doping of phosphorous in C60 structure. Mol. Struct. THEOCHEM, 624(1-3): 233-237.

Lee, Z.S.M.; (1995). AM1 stability prediction-B36N24 B36P24 Al36N24 Al36P24. Mol. Struct. THEOCHEM, 334(2-3): 229-233.

Lee, Z.S.M.; (2011). Theoretical study on the highly chlorinated smaller fullerenes of C30–C48. Comp. Theor. Chem., 967(1): 206-210.

Tang, C., *et al.*; (2012). Density functional study on the electronic properties, polarizabilities, NICS values, and absorption spectra of fluorinated fullerene derivative C60F17CF3. Comp. Theor. Chem., 991: 154-160.

Wang, Z.; Zhang, j.; (2011). DFT study on structural, electronic, and vibrational properties of the highest oxygenated fullerene C24O12. Comp. Theor. Chem., 972(1-3): 20-24.

Prinzbach, H., *et al.*; (2000). Gas-phase production and photoelectron spectroscopy of the smallest fullerene, C20. Nature, 407(6800): 60-63.

Saito, M.; Miyamoto, Y.; (2011). Theoretical identification of the smallest fullerene, C20. Phys. Rev. Let., 87(3): 035503.

Sokolova, S; Lüchow, A.; Anderson, J.B.; (2000). Energetics of carbon clusters C20 from all-electron quantum Monte Carlo calculations. Chem. Phys. Lett., 323(3–4): 229-233.

Grossman, J.C.; Mitas, L.; Raghavachari, K.; (1995). Structure and Stability of Molecular Carbon: Importance of Electron Correlation. Phys. Rev. Lett., 75(21): 3870-3873.

Grossman,J.C.; (2002). Structural isomers of C20 revisited: the cage and bowl are almost isoenergetic. Chem. Phys. Chem., 3(2): 207-209.

Brabec, C.J., *et al.*;(2015). Precursors to C60 fullerene formation. Phys. Rev. B, 46(11): 7326-7328.

Jin, Y., *et al.*, (2015). Coupled cluster geometries and energies of C20 carbon cluster isomers – A new benchmark study. Chem. Phys. Lett., 629: 76-80.

Banerjee, S.; Pillai, C.G.S.; Majumder, C.; (2011). Hydrogen absorption behavior of doped corannulene: A first principles study. Int. J. Hydrogen Energ., 36(8): 4976-4983.

Mason, J.; (1993). Conventions for the reporting of nuclear magnetic shielding (or shift) tensors suggested by participants in the NATO ARW on NMR shielding constants at the University of Maryland, College Park, Solid state nucl. magn. resonan., 2(5): 285-288.

Frisch, M., *et al.*; (1998). Gaussian 98, revision A. 7;

Gaussian, Inc. Pittsburgh, Pa, 12.

Zhang, Z.W.; Zheng, W.T.; Jiang, Q.; (2012). Hydrogen adsorption on Ce/BNNT systems: A DFT study. Int. J. Hydrogen Energ., 37(6): 5090-5099.

Galli, G.; Gygi, F.; Golaz, J.C.; Vibrational and electronic properties of neutral and negatively charged C20 clusters. Phys. Rev. B, 57(3): 1860-1867.

Fowler, P.W., *et al.*; (1991). Magnetic properties of C60 and C70. Chem. Phys. Lett., 179(1–2): 174-180.

Graybeal, J.D; (1993). Molecular Spectroscopy, McGraw-Hill, New York.

Saunders, M., *et al.*;(1996). Noble gas atoms inside fullerenes. Science, 271(5256).

Bryce, D.; Wasylishen, R.; (2000). In Encyclopedia of spectroscopy and spectrometry. Vol. 3. Edited by J.C. Lindon, G.E. Tranter, and J.L. Holmes. Academic Press, San Diego.

Ashrafi, F.G.A.; (2012). A Computational NMR Study for Chemisorption of Oxygen-doped on the Surface of Single-Walled Carbon Nanotubes. Appl. Sci., Eng. Technol, 2529-2536.

Adamo, C.; Barone,V.; (1998). Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. J. Chem. Phys., 108(2): 664-675.

Ditchfield, R.; Hehre, W.J.; Pople, J.A.; (1971). Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules. J. Chem. Phys., 54(2): 724-72.

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