AlN Nanotubes: A DFT Study of Al-27 and N-14 Electric Field Gradient Tensors

Ahmad Seif[a, b], Mahmoud Mirzaei[c], Mehran Aghaie[d], and Asadollah Boshra[a, b]

[a] Department of Chemistry, Boroujerd Branch, Islamic Azad University, Boroujerd, Iran
[b] Department of Chemistry, Science and Research Campus, Islamic Azad University, Tehran, Iran
[c] Department of Chemistry, Tarbiat Modares University, P.O. Box 14115-191, Tehran, Iran
[d] Faculty of Chemistry, North Tehran Branch, Islamic Azad University, Tehran, Iran

Reprint requests to M. M.; E-mail: mirzaei_md@yahoo.com

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Density functional theory (DFT) calculations were performed to calculate the electric field gradient (EFG) tensors at the sites of aliminium (^{27}Al) and nitrogen (^{14}N) nuclei in an 1 nm of length (6,0) single-walled aliminium nitride nanotube (AlNNT) in three forms of the tubes, i. e. hydrogen-capped, aliminium-terminated and nitrogen-terminated as representatives of zigzag AlNNTs. At first, each form was optimized at the level of the Becke3,Lee-Yang-Parr (B3LYP) method, 6-311G** basis set. After, the EFG tensors were calculated at the level of the B3LYP method, 6-311++G** and individual gauge for localized orbitals (IGLO-II and IGLO-III) types of basis sets in each of the three optimized forms and were converted to experimentally measurable nuclear quadrupole resonance (NQR) parameters, i. e. quadrupole coupling constant (qcc) and asymmetry parameter (η_Q). The evaluated NQR parameters revealed that the considered model of AlNNT can be divided into four equivalent layers with similar electrostatic properties. With the exception of Al-1, all of the three other Al layers have almost the same properties, however, N layers show significant differences in the magnitudes of the NQR parameters in the length of the nanotube. Furthermore, the evaluated NQR parameters of Al-1 in the Al-terminated form and N-1 in the N-terminated form revealed the different roles of Al (base agent) and of N (acid agent) in AlNNT. All the calculations were carried out using the GAUSSIAN 98 package program.

Key words: Aluminium Nitride; Nanotube; DFT; NQR; Electric Field Gradient.