# A Nano-motor Simulation of $B_nN_n$ (Rotor) and $BN^{(-,0,+)}$ B (stator) Applying for Detecting Biological Molecules in IR Regions

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**Abstract:** We have shown the $BN^{(-,0,+)}$ B-$B_nN_n$ system works as a quantum rotatory machine which has a range of spectrum in the IR region caused by the alternative attraction and repulsion forces. The electromagnetic non-bonded interactions of $BN^{(-,0,+)}$ B systems (working as quantum stator) inside several $B_nN_n$ molecular rings (as a rotor) has been investigated using EPR-II and EPR-III basis sets

Double minimum of the BNB potential well is due to the lack of correct permutational symmetry of its wave function and charge distribution. In this study, it has been indicated that through the interaction of BNB (both radical and cation) with $B_nN_n$, the energy barrier in SB effect increases dramatically compared to when the BNB is isolated. In terms of intermolecular forces, whether the systems of $B_2N^{(0,-,+)}$ are open shell or closed shell, the interaction is either repulsive or attractive. The latter depends both on the diameter of $B_nN_n$ rings and whether the system is ionic or radical. Optimized structures as well as relative stability of the system and the hyperfine spectroscopic parameters have been calculated. It has been indicated in this study that the $B_nN_n$–BNB systems can work as a nano rotor-stator machine (similar to a molecular motor system) in biological systems. Although the NMR, stability and electromagnetic properties of a few models of $B_nN_n$ rings have been discussed in our previous studies [1-5], employing such system as a detector is much more significant and can be investigated for further studies.

Extensive calculations have been carried out on the radical, anionic and cationic forms of $BH_2NBH_2$ to obtain data and it has been observed that the radial coordinate of the dipole moment vector (r) as well as the voltage differences ($\Delta$V) and relative energies ($\Delta$E) exhibited Gaussian distribution. We have obtained a relationship between dipole moments and the voltage differences and energies of system.

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