

## The value of NMR parameters and DFT calculations for Quantum Information Processing utilizing Phosphorus Heterocycles

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Abstract: Quantum computing is the field of science that uses quantum-mechanical phenomena, such as superposition and entanglement, to perform operations on data. The fundamental information unit used in quantum computing is the quantum bit or qubit [1-2]. The principal difference between a qubit and a classical computing bit is: A quantum bit can be in any of a potentially infinite number of states and quantum systems can be simultaneously in superposition with many of the basis states [2]. That makes the computational basis vastly increased, because a series of operations can be performed nearly simultaneously; and, theoretically, solve problems much more quickly than any classical computers [2-3]. Currently, the first and still the most successful implementations of quantum information processing (QIP) have been based on nuclear spins in liquids [3]. However, molecules that enable many qubits NMR OIP implementations should meet some conditions: have large chemical shifts and be appropriately dispersed for qubit addressability, appreciable spin-spin coupling between any pair of spins, and a long relaxation time [4]. In this line, Benzyldene-2,3-dihydro-1H-[1,3]diphosphole (BDF) derivatives have been theoretically tested for maximizing large chemical shifts, spin-spin coupling, and minimizing the hyperfine coupling constant. The NMR spectroscopic parameters ( $\delta$  and J) were calculated with six different DFT functionals. The  $\tau$ -HCTH/6-31G(2d) level is in better agreement with the experimental data of <sup>31</sup>P and <sup>13</sup>C chemical shifts. While PCM-B3LYP/cc-pVDZ level shows a decrease on deviation between calculated and experimental values for NMR properties. Finally, the Surface Response technique was employed to rationalize how the hyperfine constant varies with the chemical shifts and coupling constants values. From our findings, BDF-NO<sub>2</sub> was the best candidate for NMR quantum computations (NMR-QC) among the studied series.

Key-words: <sup>31</sup>P NMR, NMR parameters calculations, quantum computation

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