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Theoretical studies on the potentials of some nanocages (Al₁₂N₁₂, Al₁₂P₁₂, B₁₂N₁₂, Be₁₂O₁₂, C₁₂Si₁₂, Mg₁₂O₁₂ and C₂₄) on the detection and adsorption of Tabun molecule: DFT and TD-DFT study



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Theoretical studies on the potentials of some nanocages ($\text{Al}_{12}\text{N}_{12}$, $\text{Al}_{12}\text{P}_{12}$, $\text{B}_{12}\text{N}_{12}$, $\text{Be}_{12}\text{O}_{12}$, $\text{C}_{12}\text{Si}_{12}$, $\text{Mg}_{12}\text{O}_{12}$ and C_{24}) on the detection and adsorption of Tabun molecule:

DFT and TD-DFT study

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