

PEP Vibrations from DFT

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Phosphoenol pyruvate (PEP) was studied as fully ionized, singly protonated and doubly protonated in gas-, H₂O- and D₂O-phase using density functional theory (DFT) with the B3LYP functional and with the 6-31++G(d,p) basis set. All computations except the gas-phase were compared with experimental Fourier transform infrared (FTIR) results in solution and were in good agreement. The P-O stretching is of specific importance since phosphate is transferred from PEP to adenosine diphosphate (ADP) in the glycolytic pathway. The computational assignments of these specific frequencies are provided.