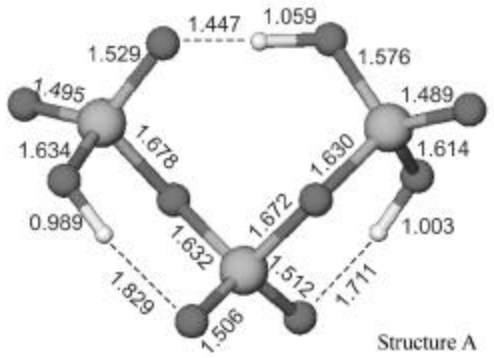
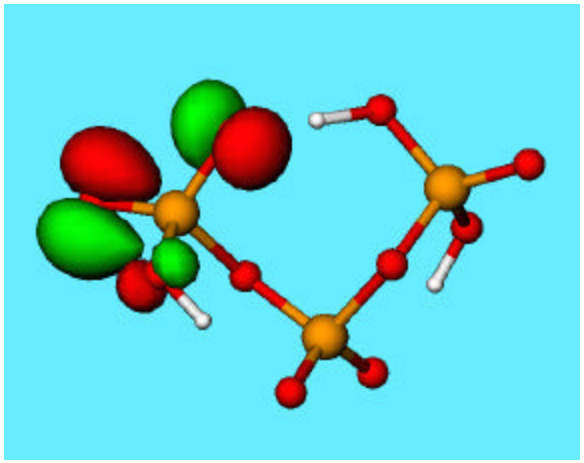
Pilot-CSD2 Highlight

WSU, EMSL

Pyrophosphate Dianions





The pyrophosphate linkage P-O-P plays an essential role in biology and is the main structural form through which energy is transmitted within living cells. In the physiological pH range the pyrophosphate and adenosine triphosphate (ATP) have two to three negative charges. We report a combined experimental and theoretical investigation on the dihydrogen phosphate anion ($H_2PO_4^-$) and two common pyrophosphate dianions, $H_2P_2O_7^{2-}$ and $H_3P_3O_{10}^{2-}$, as well as the corresponding neutral and singly-charged species.
The .global minimum structure and the HOMO of $H_3P_3O_{10}^{2-}$ are shown here.

Reference:

"Experimental and Theoretical Investigations of the Stability, Energetics, and Structures of $H_2PO_4^-$, $H_2P_2O_7^{2-}$, and $H_3P_3O_{10}^{2-}$ in the Gas Phase" X. B. Wang, E. R. Vorpagel, X. Yang, and L. S. Wang, J. Phys. Chem. A in press