A Friday Synthesis Symposium Presentation:
Flexibility of Carbodiphosphorane, C(PPh₃)₂, and it’s Reactivity Toward Main Group and Transition Metals

Speaker: Patrick Quinlivan (Parkin Group)

When: Friday, March 3rd, 2017 at 4:00 PM

Where: 209 Havemeyer

Abstract: Despite being known since 1961, there has been a recent revival of carbodiphosphoranes, C(PR₃)₂. An interesting feature of C(PR₃)₂ is that the carbon atom is formally zerovalent and possesses two lone pairs of electrons, such that the geometry is bent. However, we have demonstrated that C(PPh₃)₂ can exist in a linear form, thus providing evidence for its flexible nature.

The bonding within C(PPh₃)₂ has been examined by density functional theory calculations which demonstrate that the energy surface for bending the P–C–P bonds is very shallow. In view of the presence of the lone pairs on carbon, C(PPh₃)₂ may serve as a ligand for a variety of main group and transition metals, which will be elaborated upon in this Friday Synthesis Symposium.