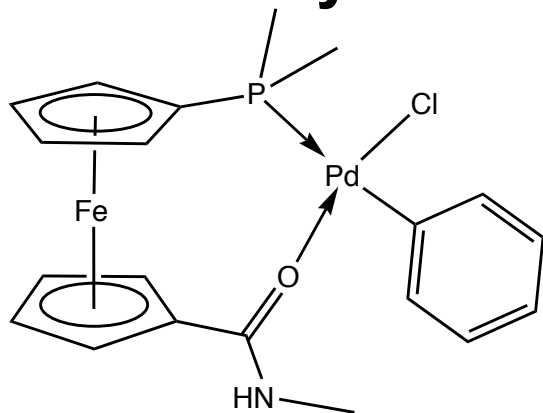
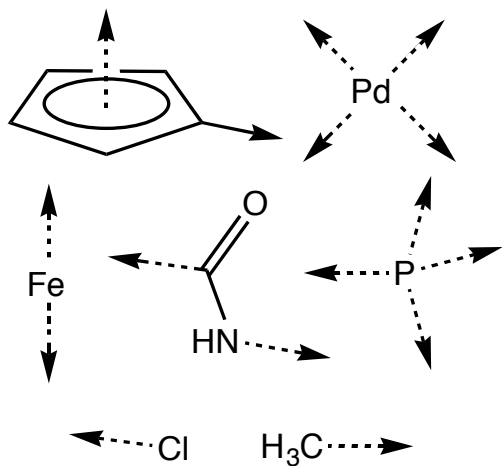


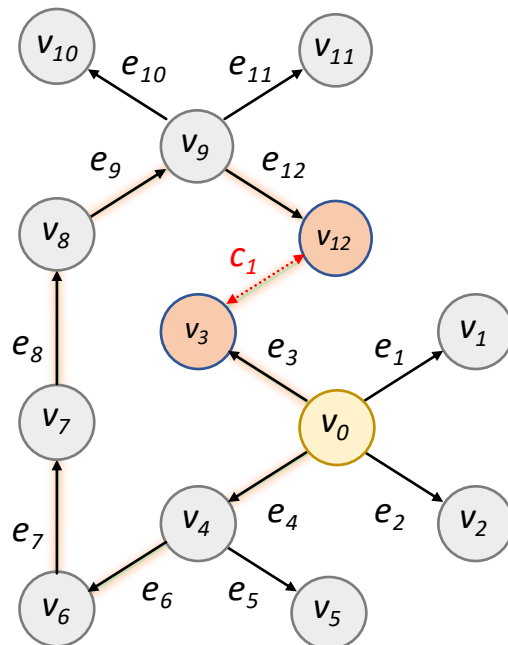
## Chemical entity:



## Fragments:



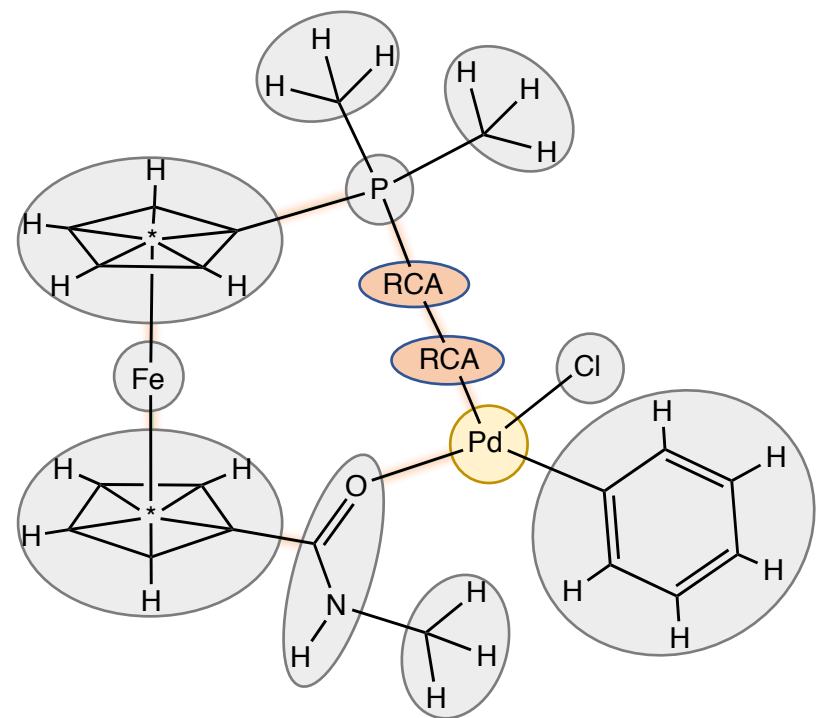
## Outer Graph:



Spanning tree:  $T(V, E)$   
 $V = \{v_1 \dots v_n\}$  fragments  
 $E = \{e_1 \dots e_n\}$  connections

Fundamental cycles  
 $Fc = \{c_1 \dots c_n\}$

## Inner Graph:



Atoms and bonds.  
 Gateway to conventional  
 representations and  
 identifiers.