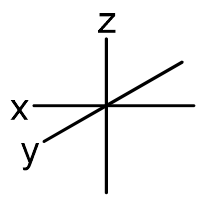
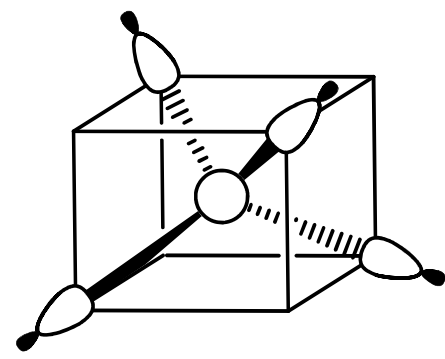


Construction of SALCs for σ bonding in T_d complexes

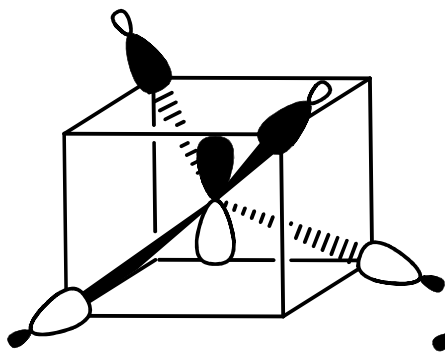
$$\Gamma_{\sigma} = A_1 + T_2$$



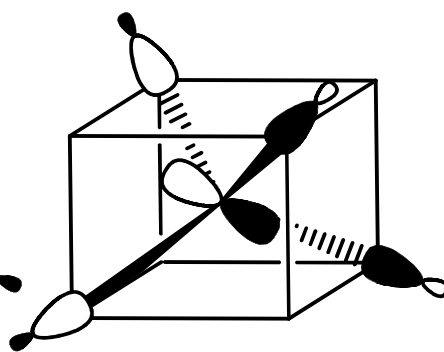
A_1
(0 nodes)



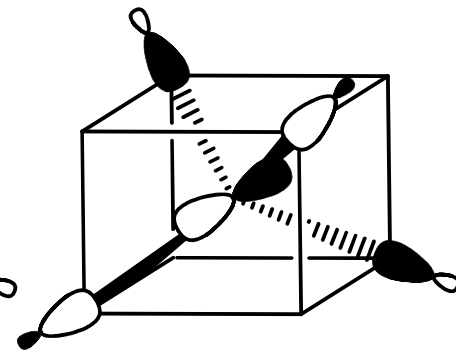
T_2
(1 node)



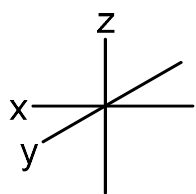
p_z



p_x



p_y



$$\Gamma_{\sigma} = A_1 + T_2$$

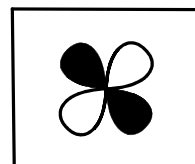
AOs



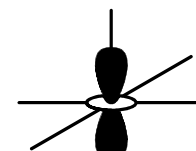
d_{xy}



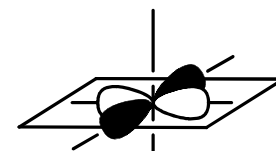
d_{yz}



d_{xz}



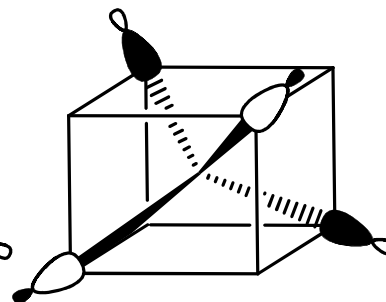
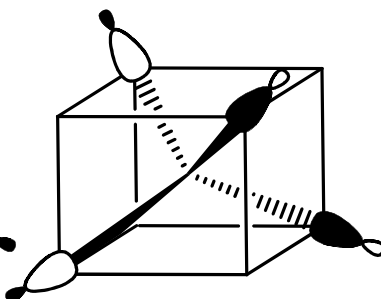
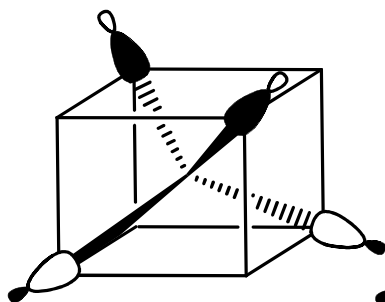
d_{z^2}



$d_{x^2-y^2}$

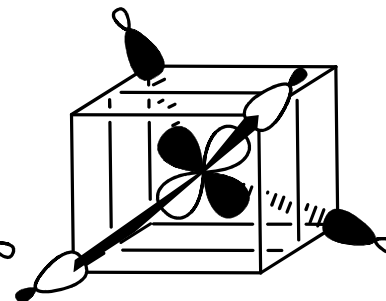
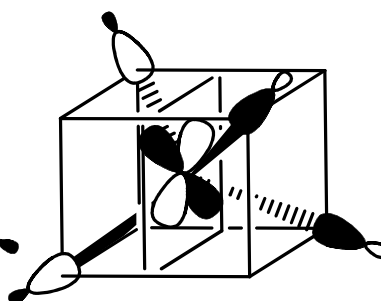
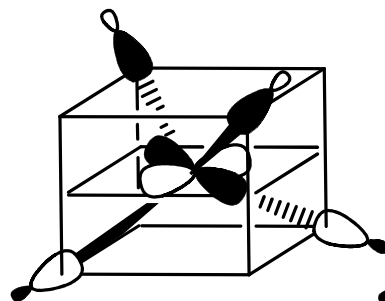
SALCs

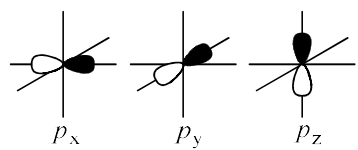
T_2
(1 node)



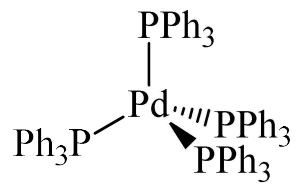
MOs

T_2
(1 node)

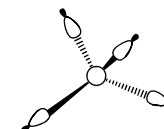
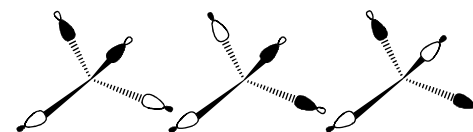
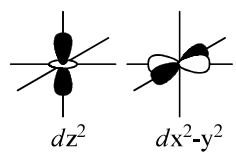
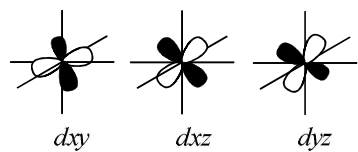
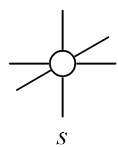


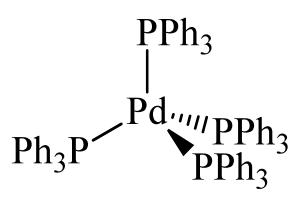
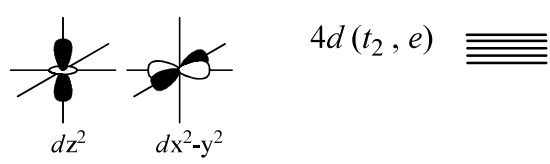
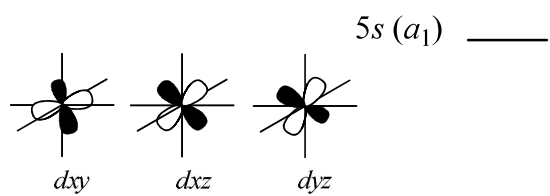
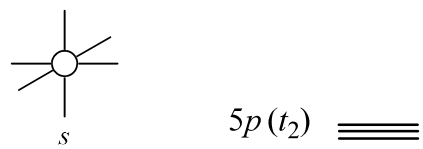
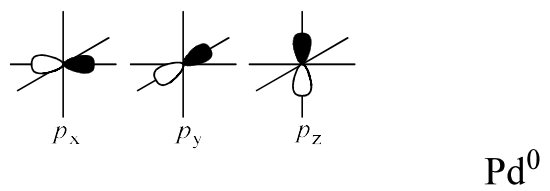


Pd^0

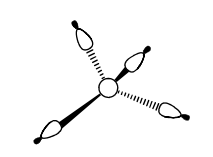
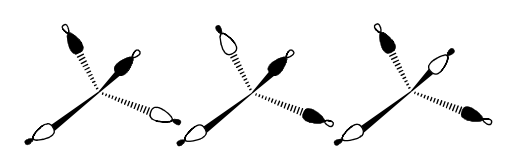


4 PPh_3



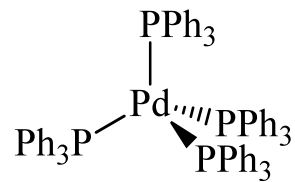
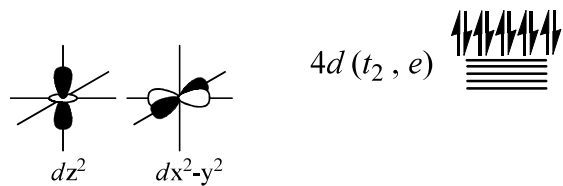
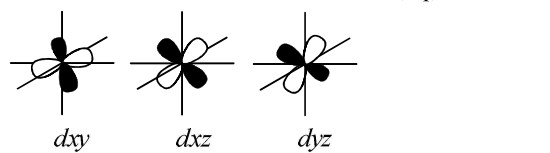
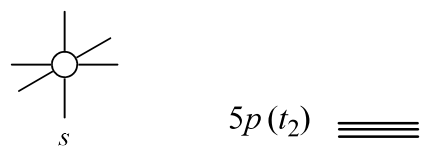
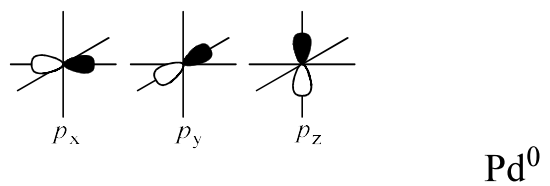


4 PPh_3

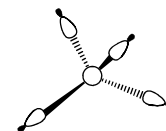


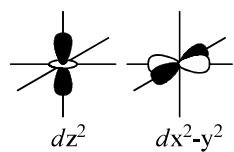
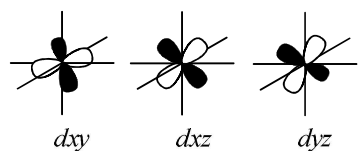
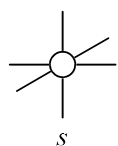
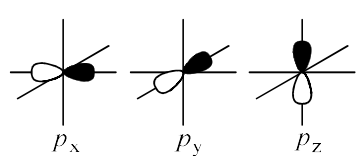
$\equiv \equiv \equiv$ t_2

--- a_1

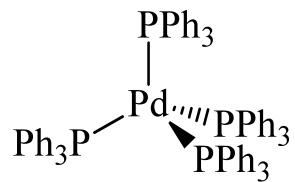


4 PPh_3





Pd^0



4 PPh_3

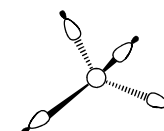
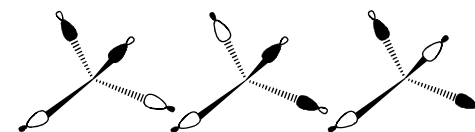
$5p(t_2)$

$5s(a_1)$

$4d(t_2, e)$

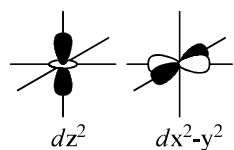
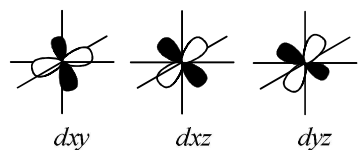
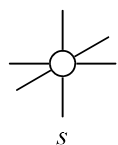
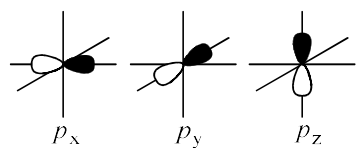
a_1^*

a_1

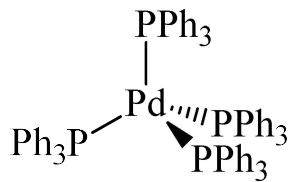


t_2

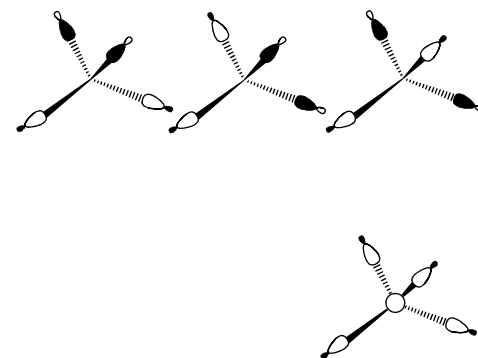
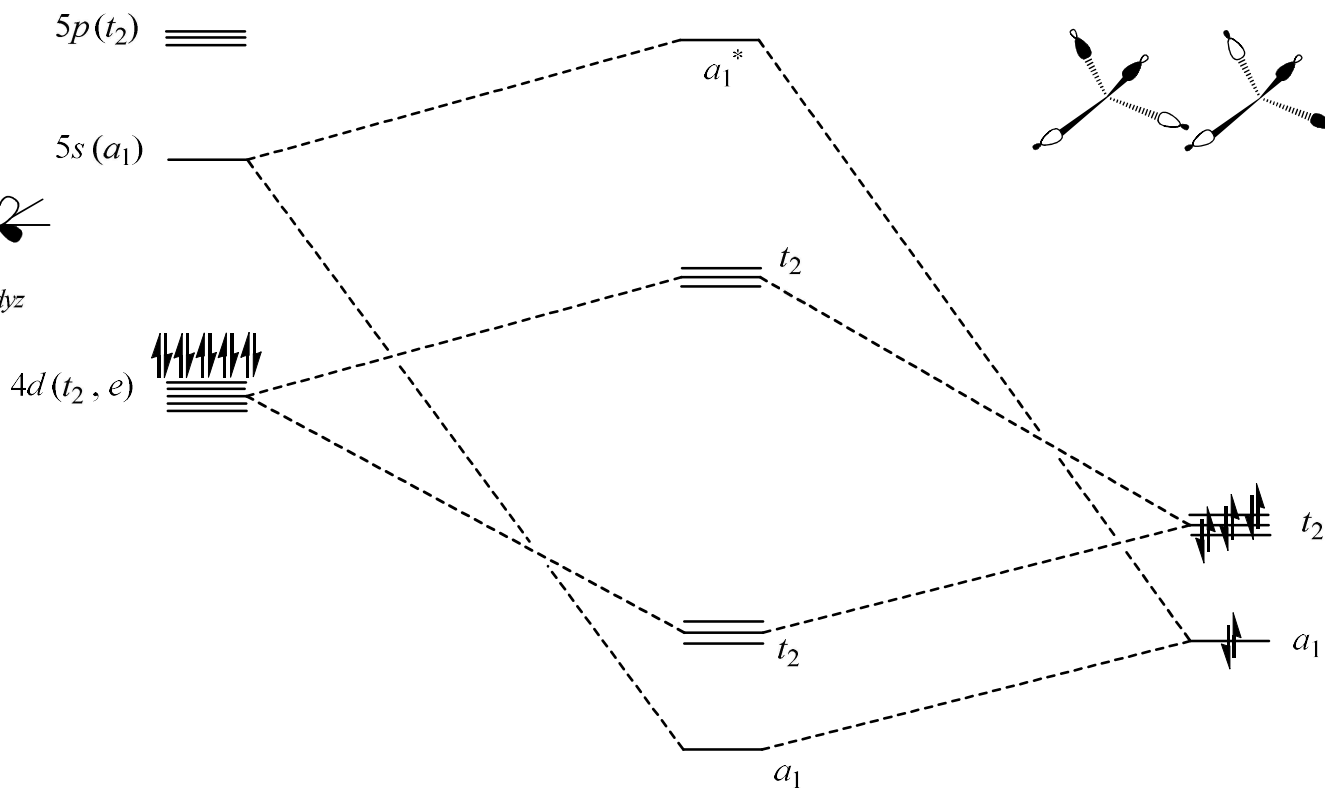
a_1

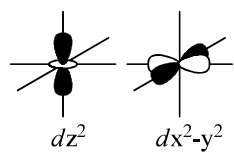
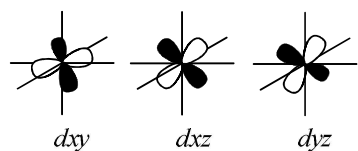
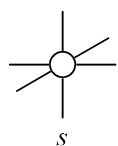
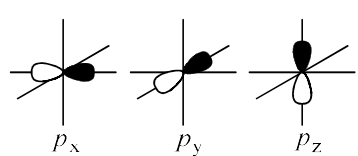


Pd^0

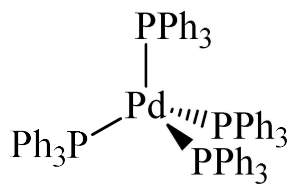


4PPh_3

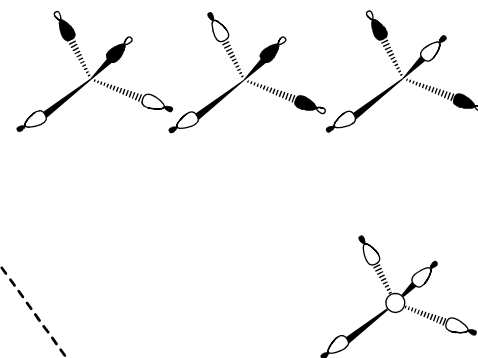
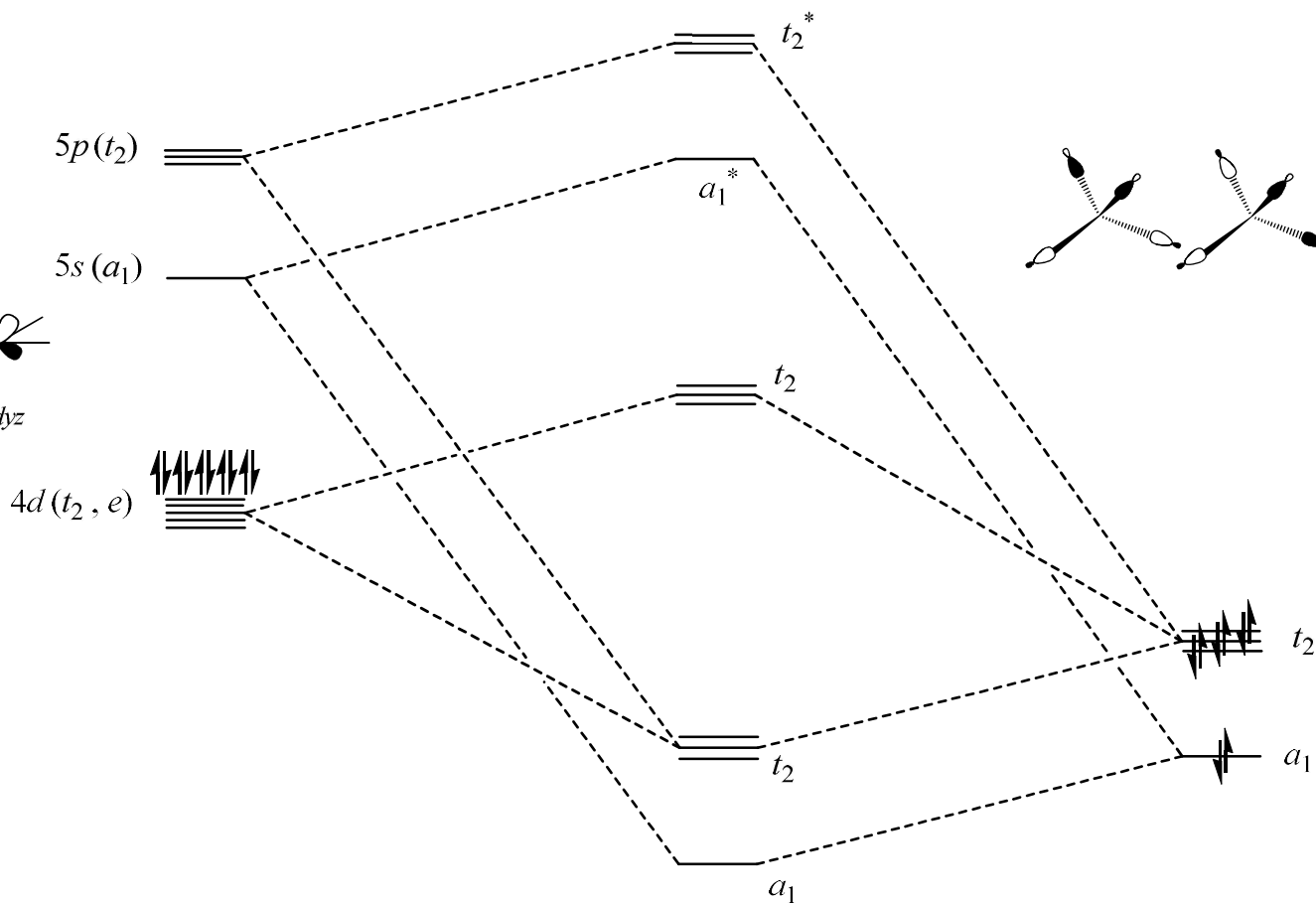


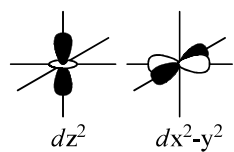
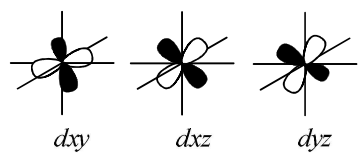
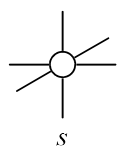
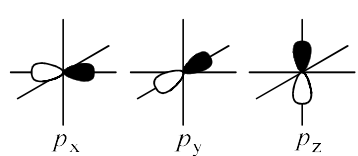


Pd^0

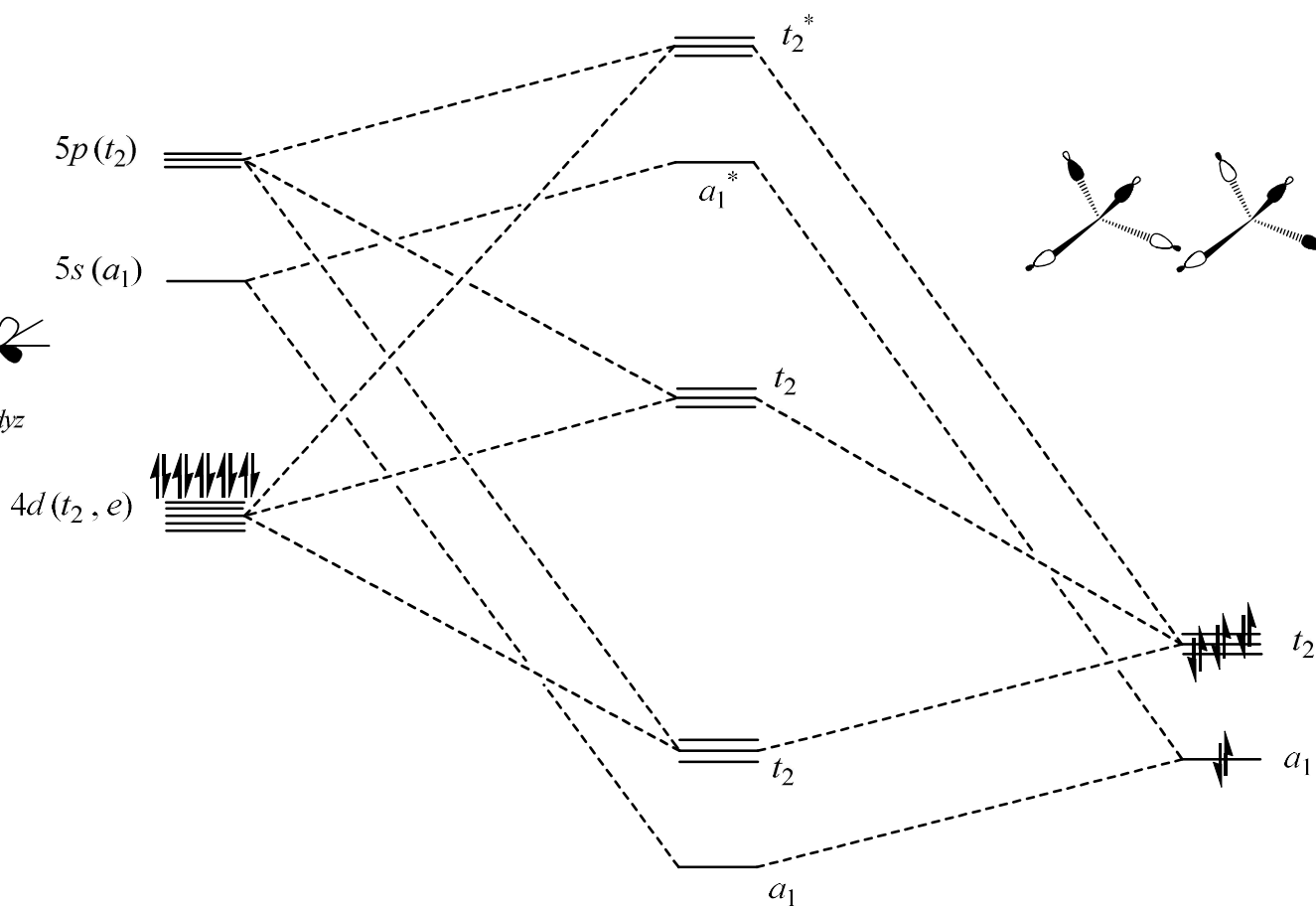
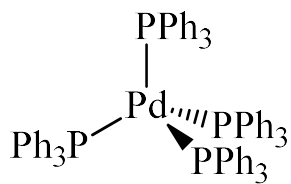


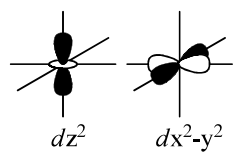
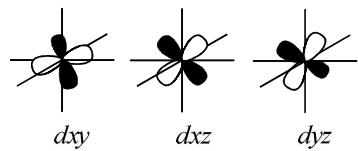
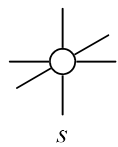
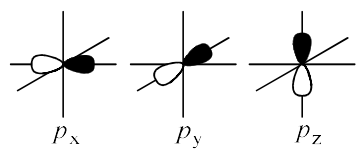
4 PPh_3



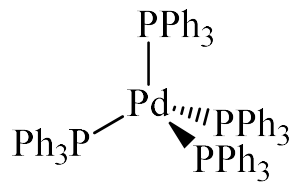


Pd^0

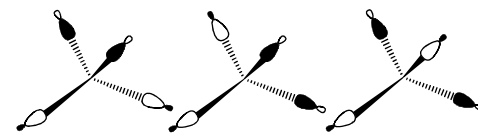
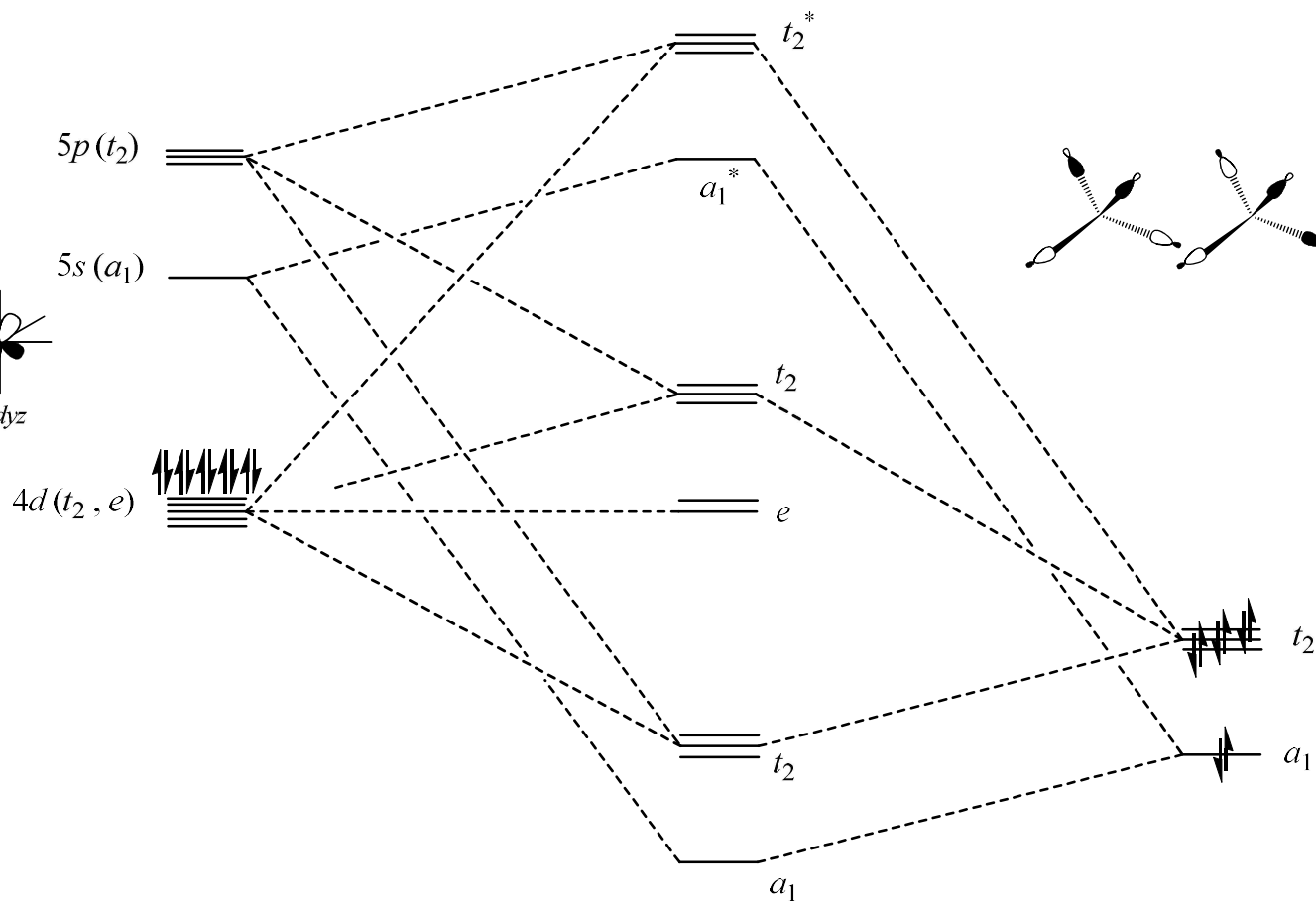


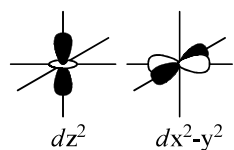
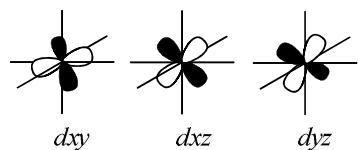
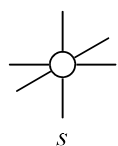
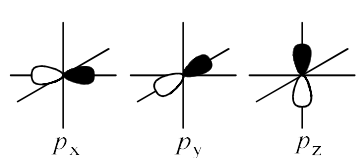


Pd^0

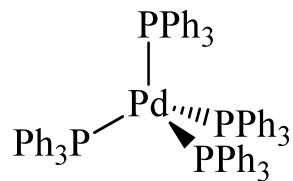


4 PPh_3

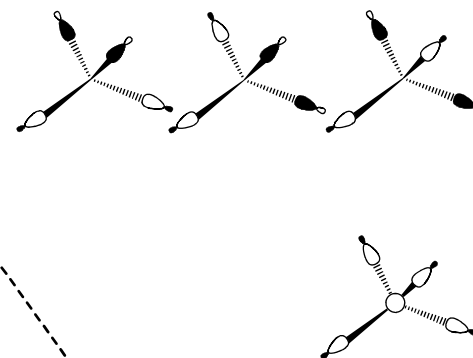
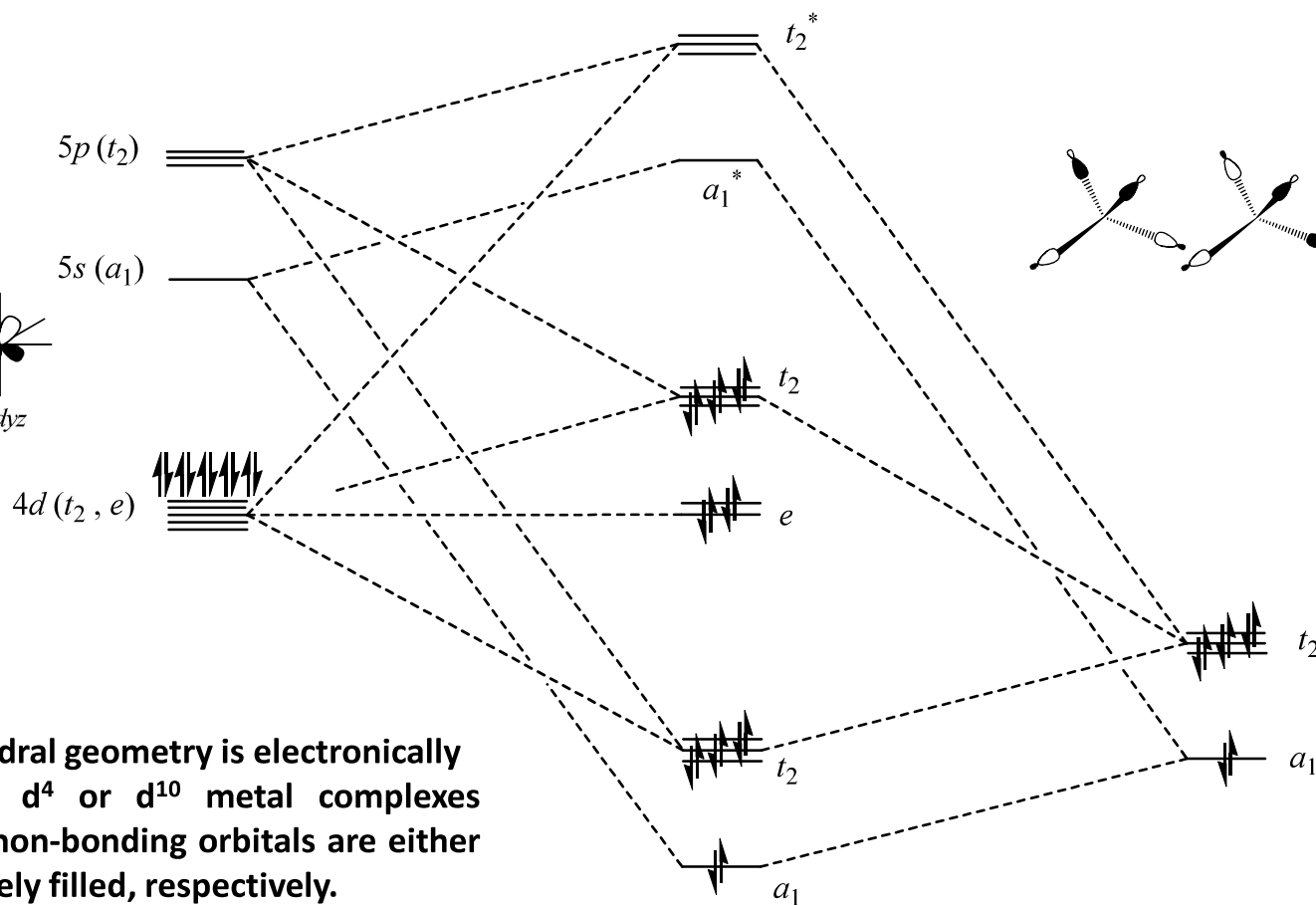




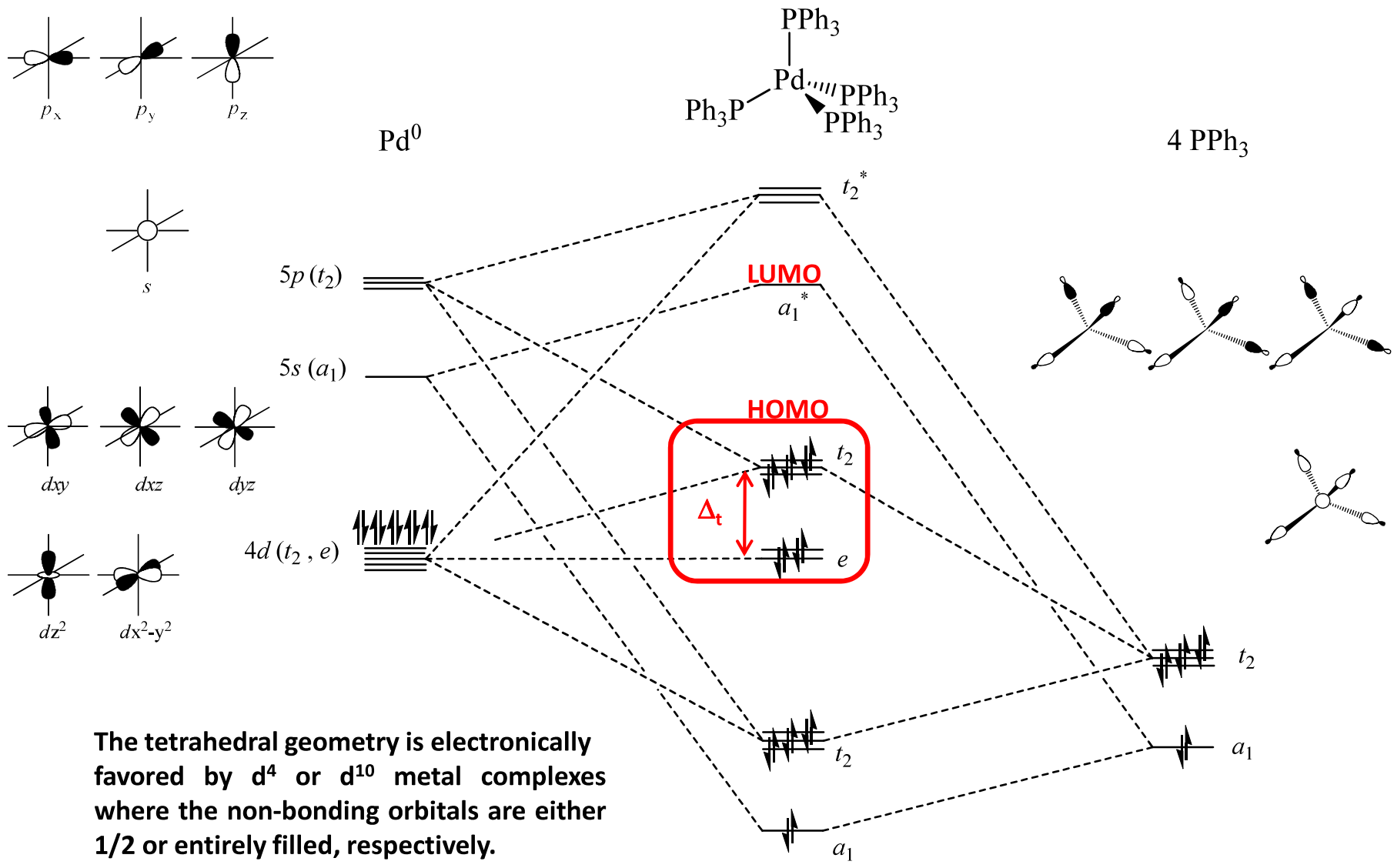
Pd^0



4 PPh_3



The tetrahedral geometry is electronically favored by d^4 or d^{10} metal complexes where the non-bonding orbitals are either 1/2 or entirely filled, respectively.



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