Investigations on the Reduction of Aldehydes by a Pyridone Borane Complex

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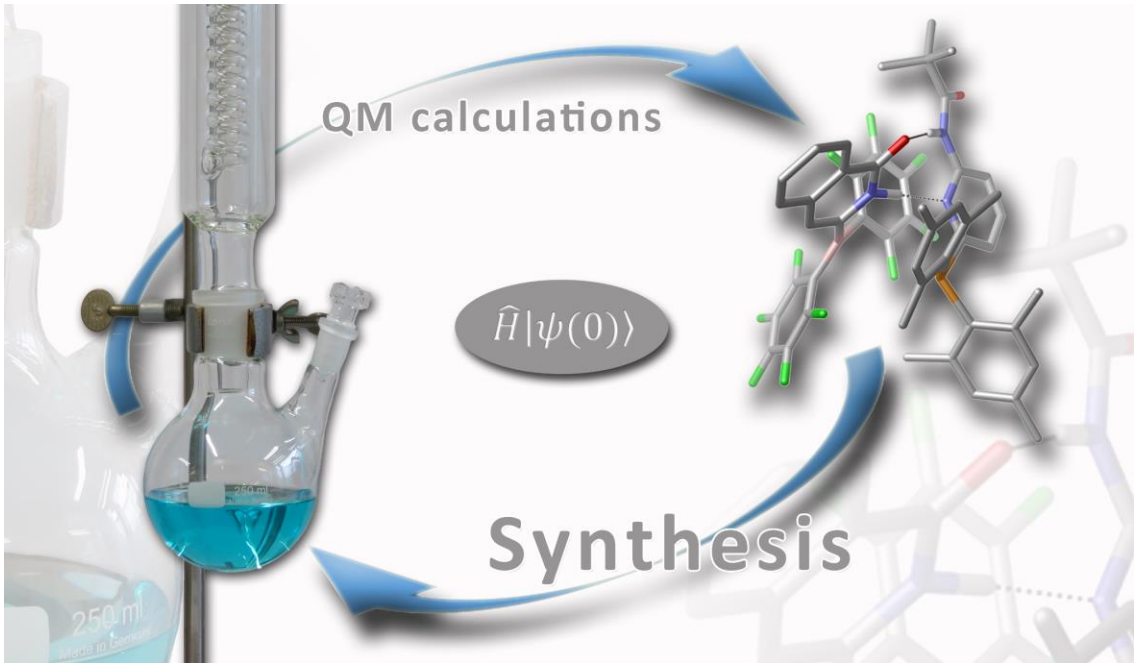
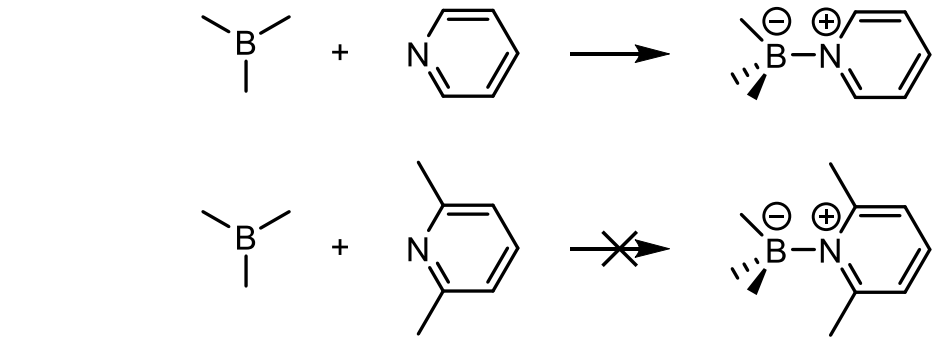
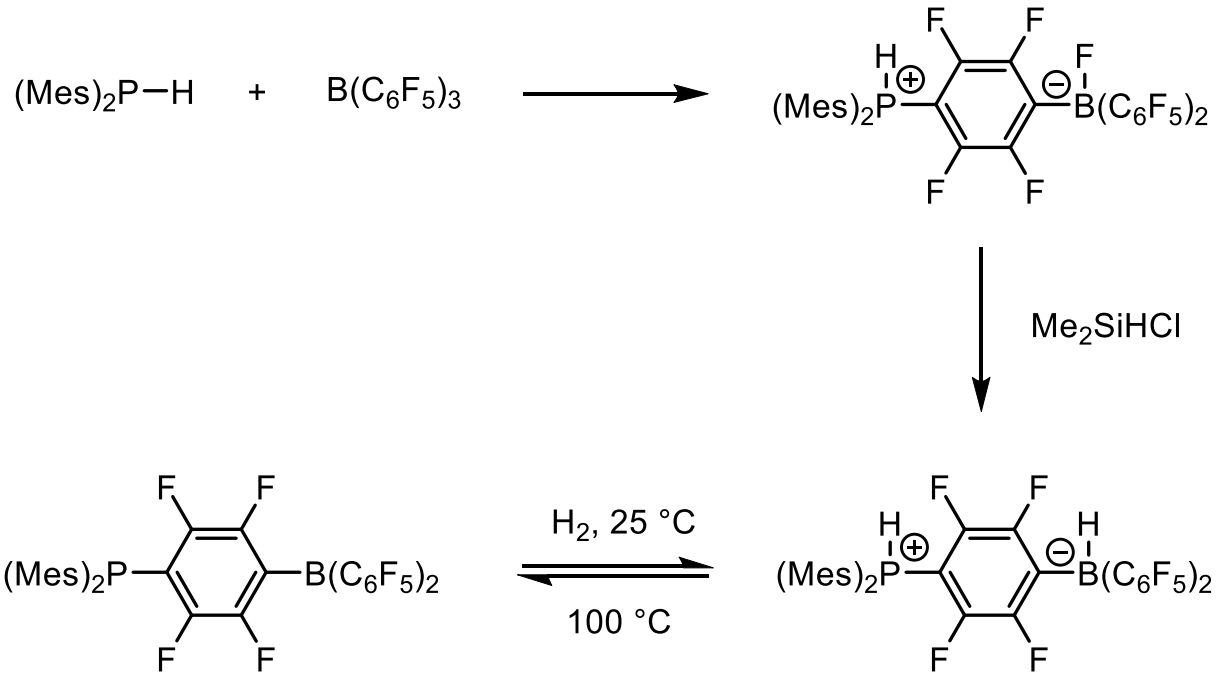


Frustrated Lewis Pairs





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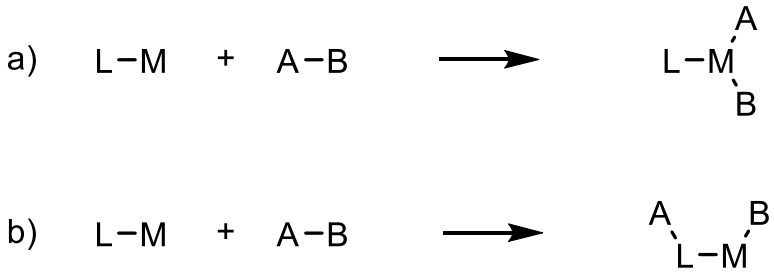
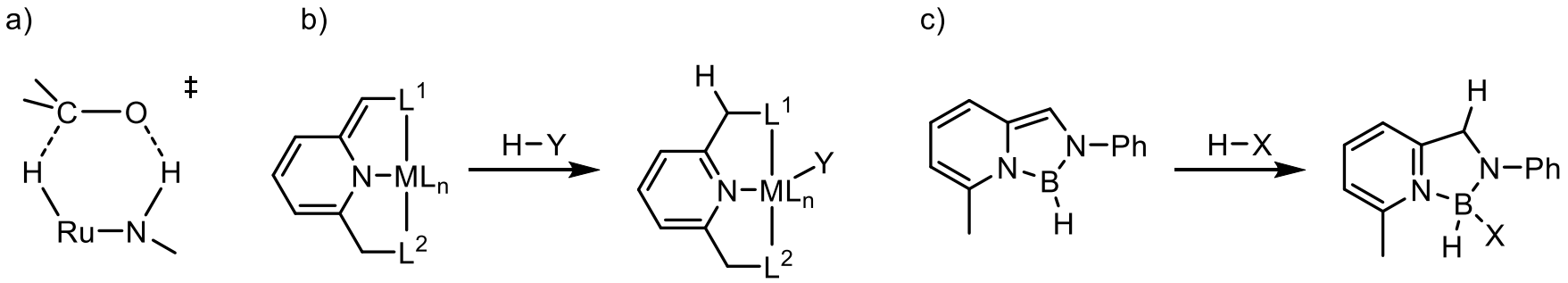
Ligand cooperation





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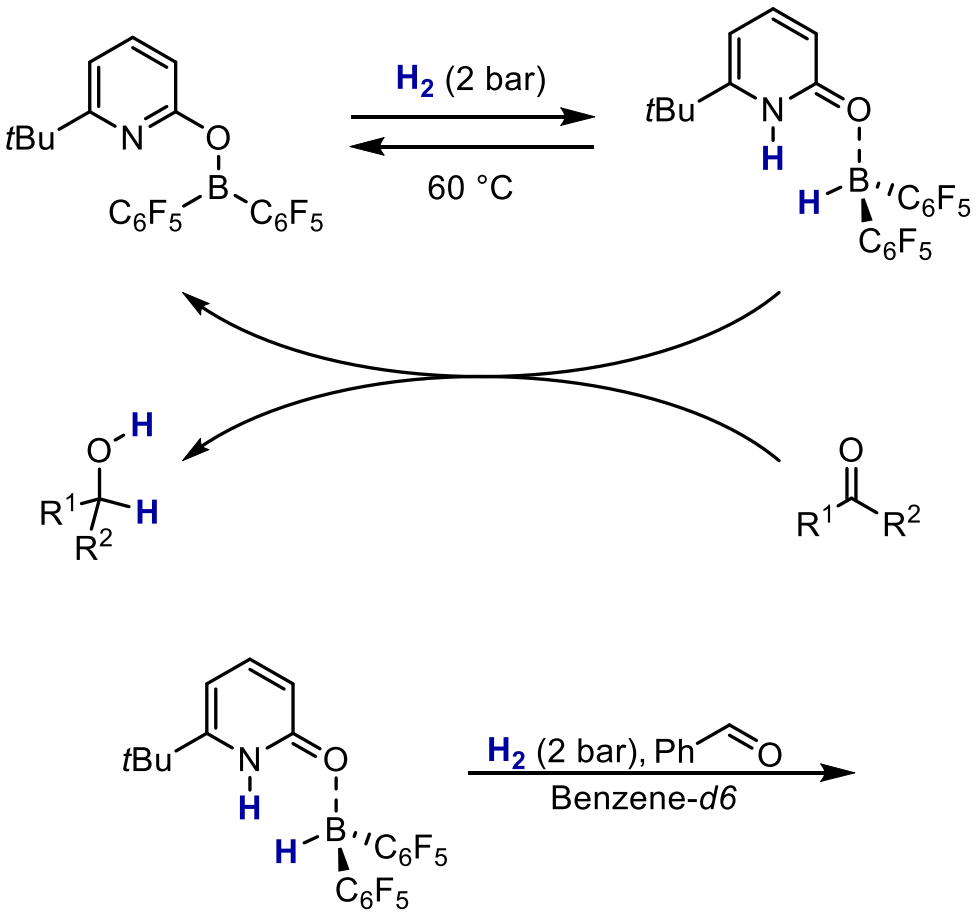
Motivation



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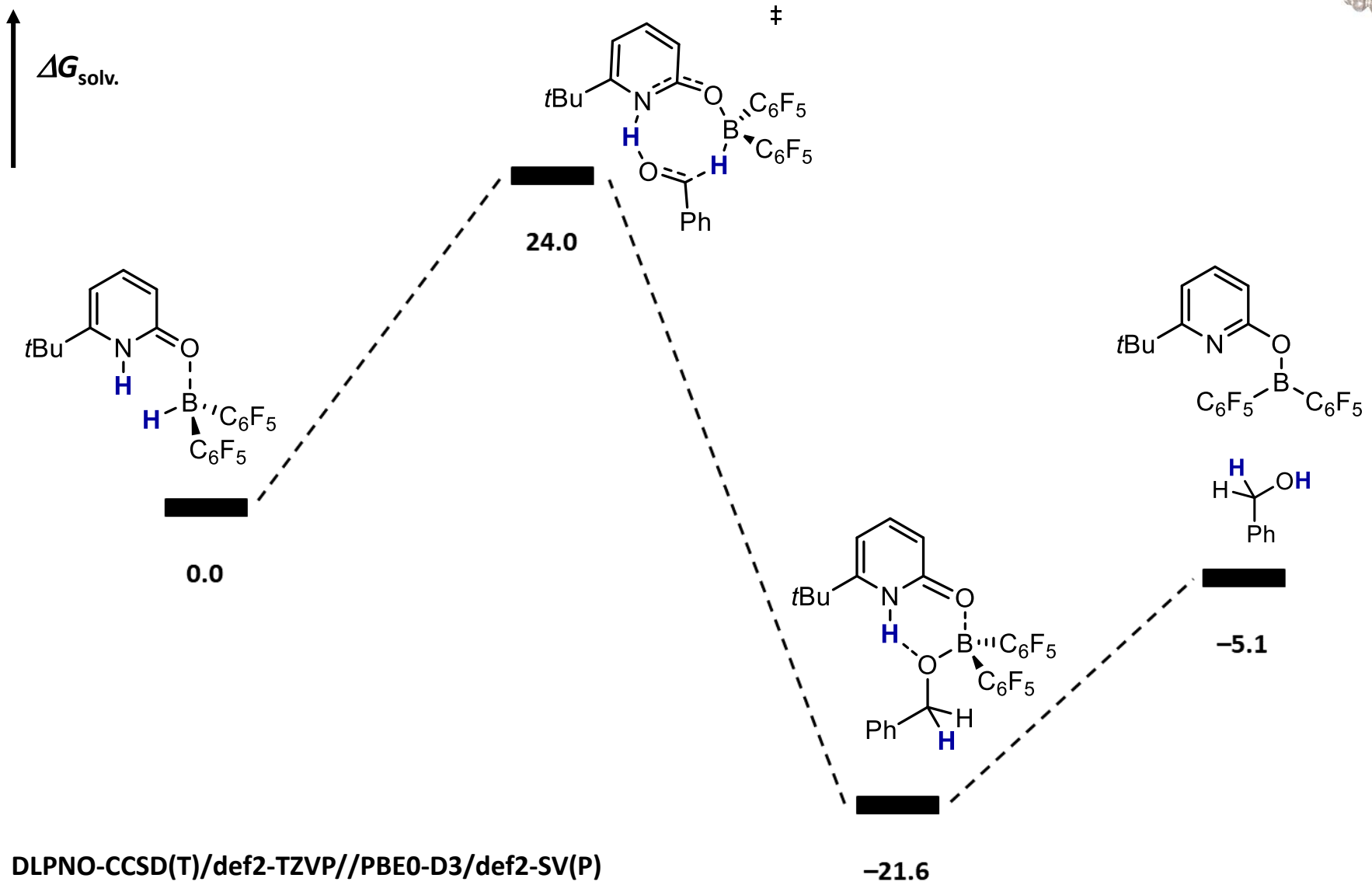
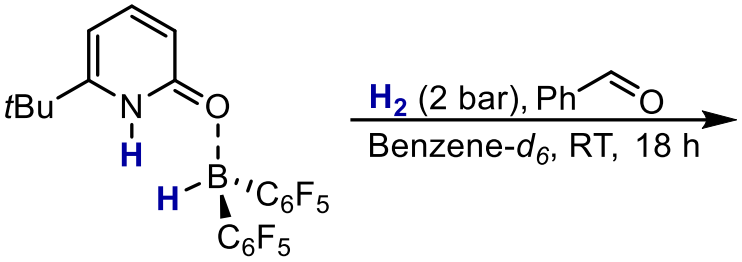
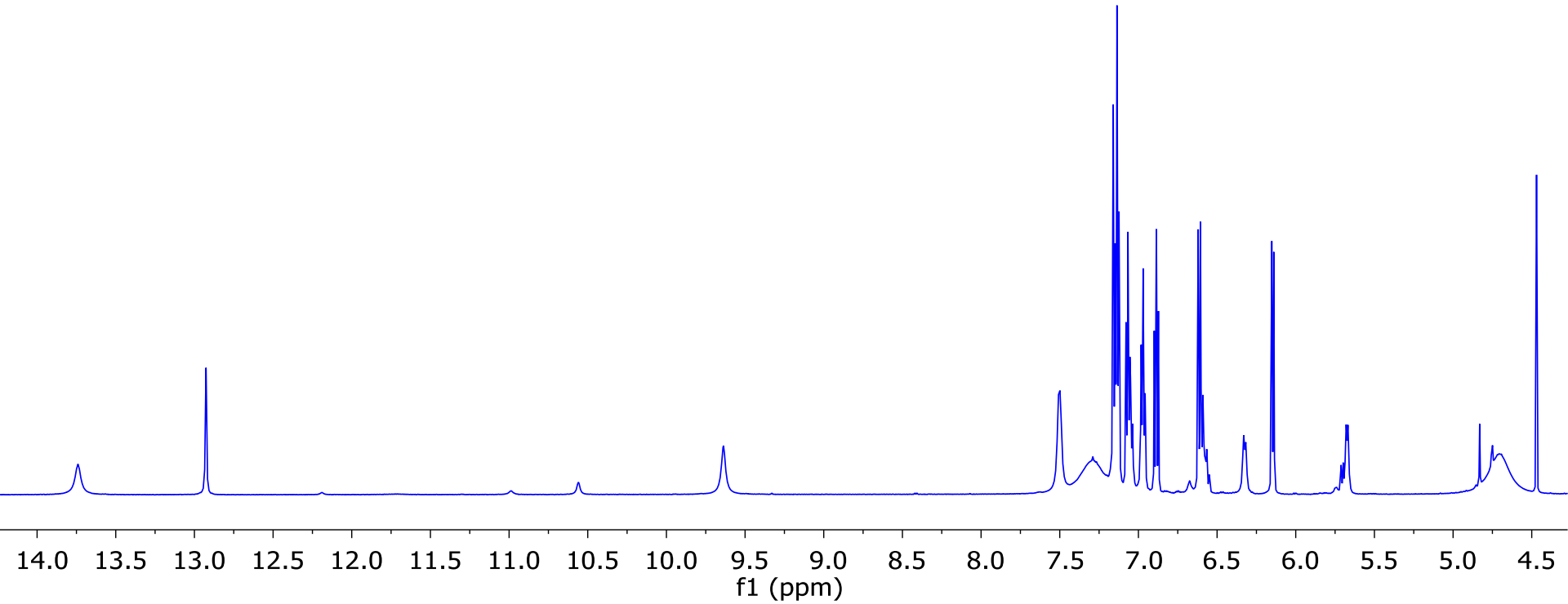
Reduction of Benzaldehyde: PES



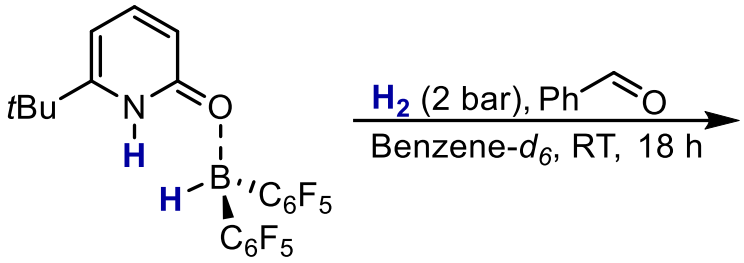
DLPNO-CCSD(T)/def2-TZVP//PBE0-D3/def2-SV(P)
SMD: Benzene

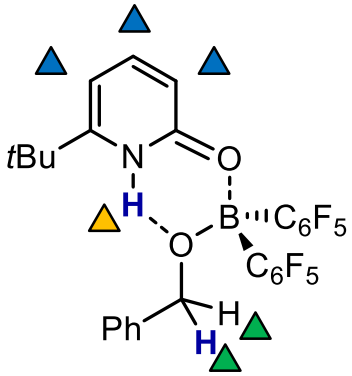
Deciphering the Reaction

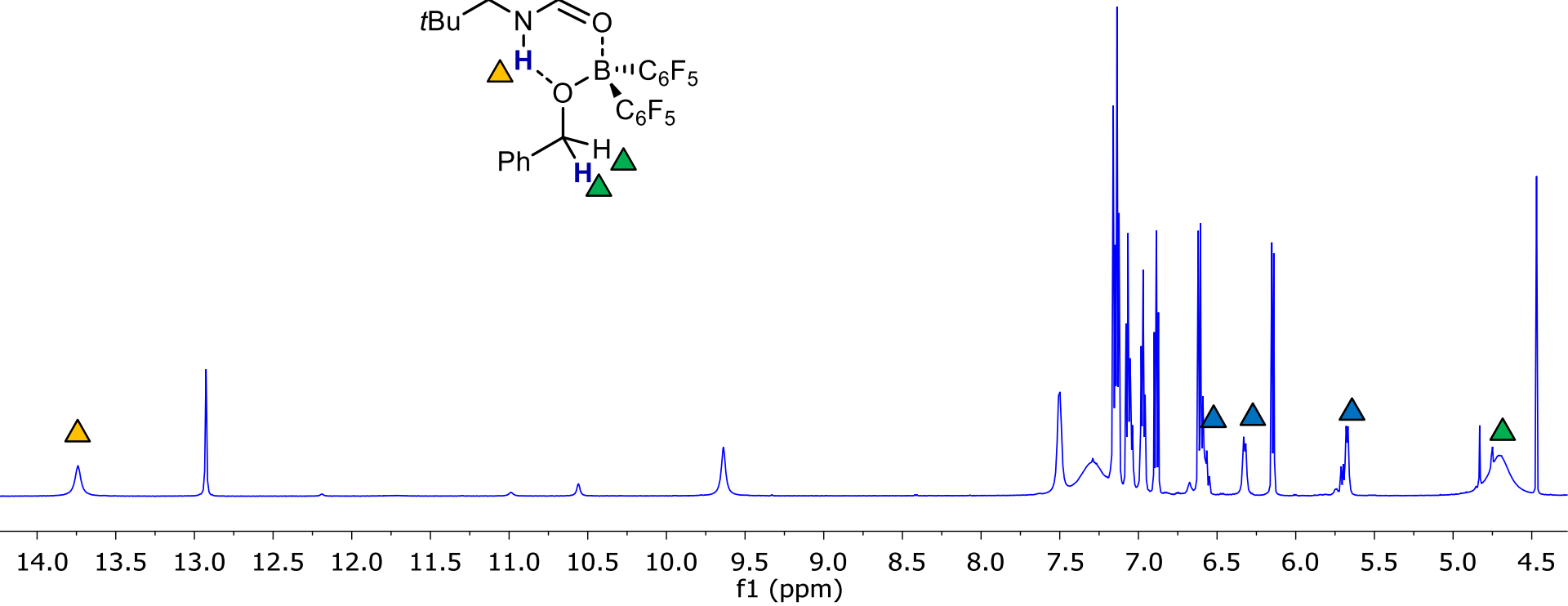




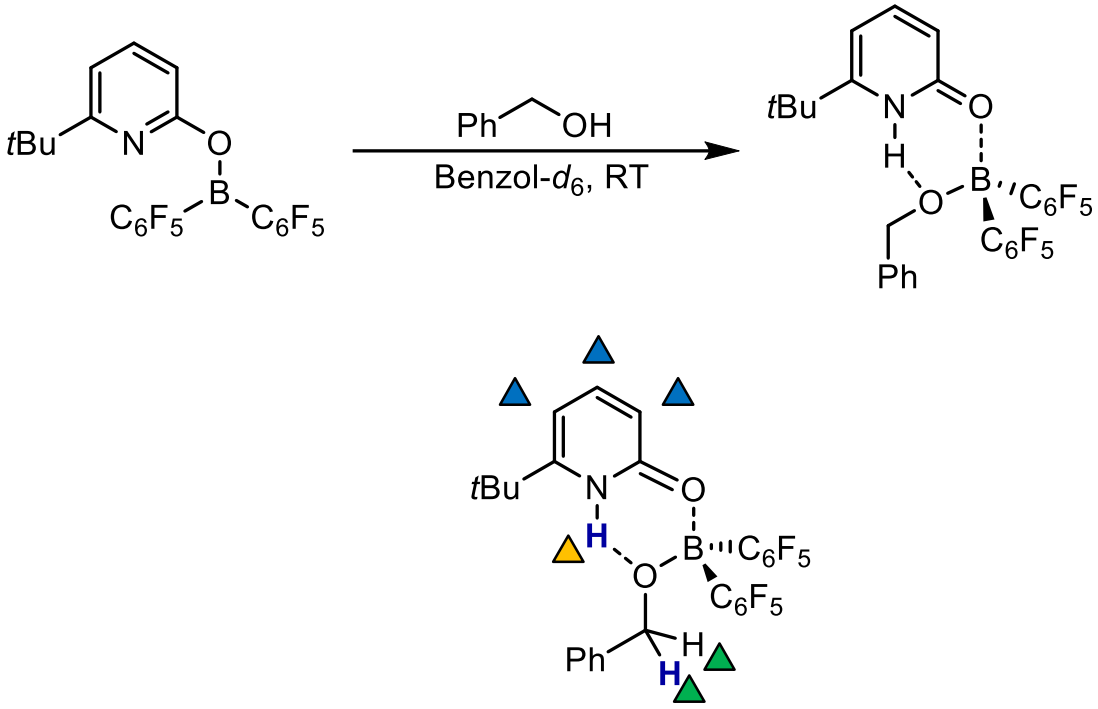
Deciphering the Reaction I

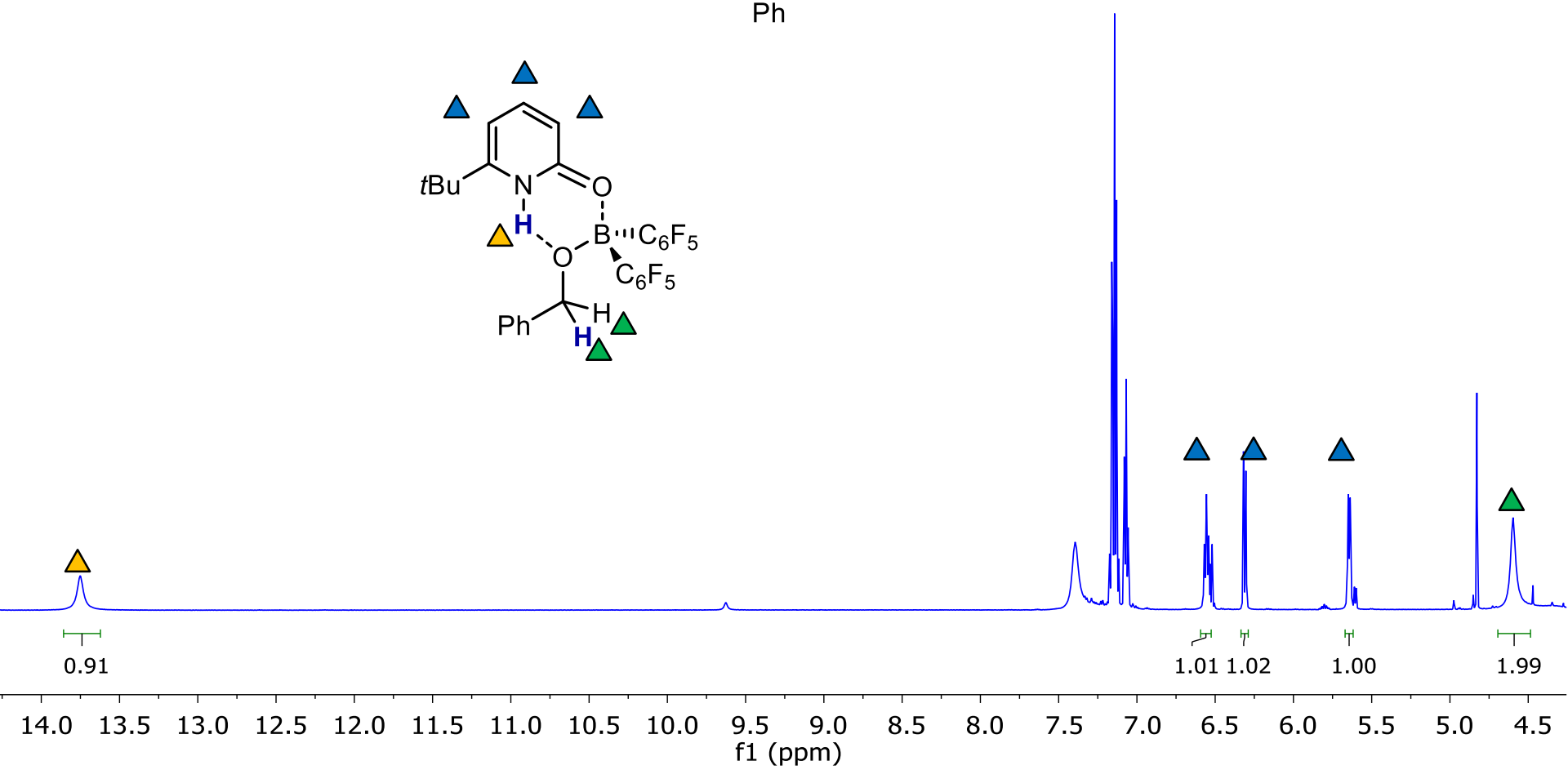






Deciphering the Reaction I





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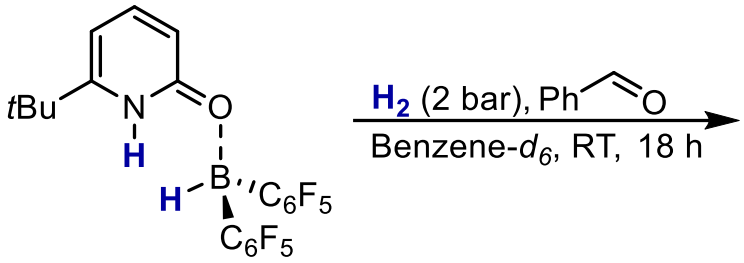

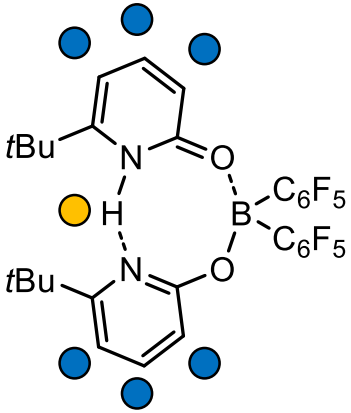

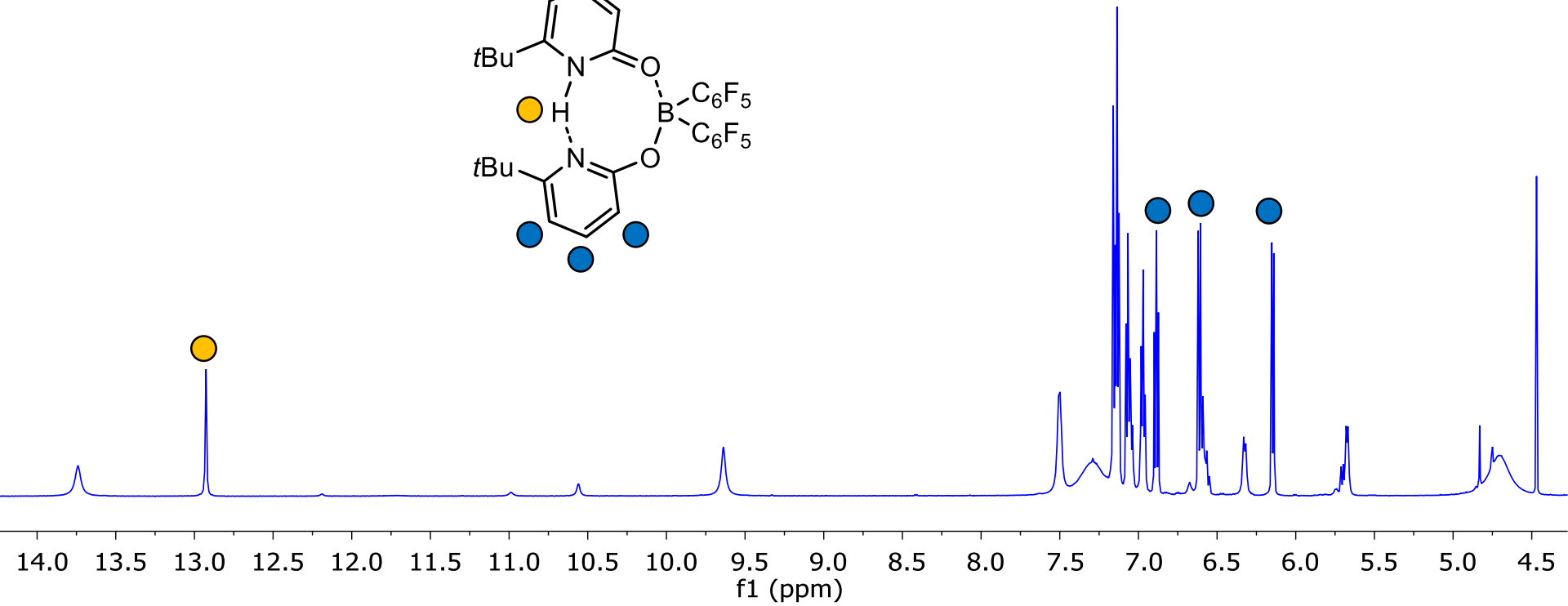

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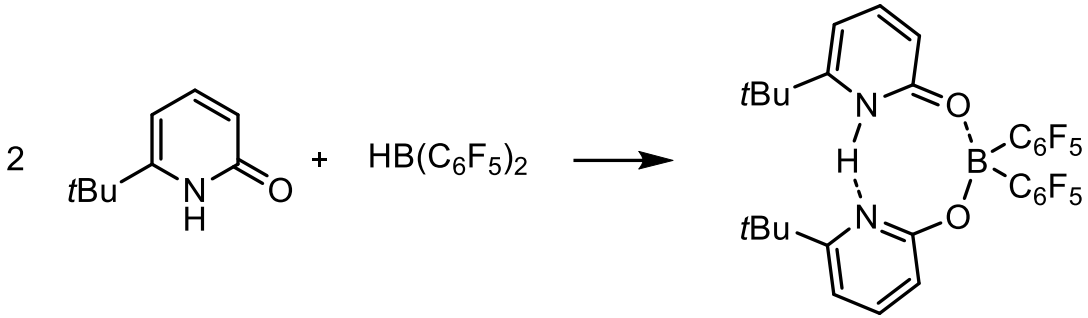

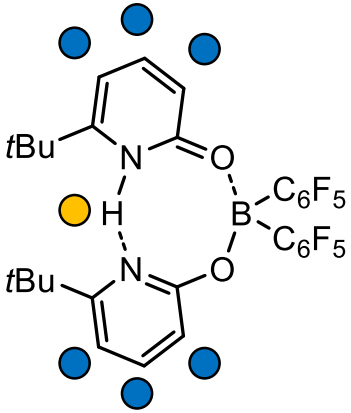

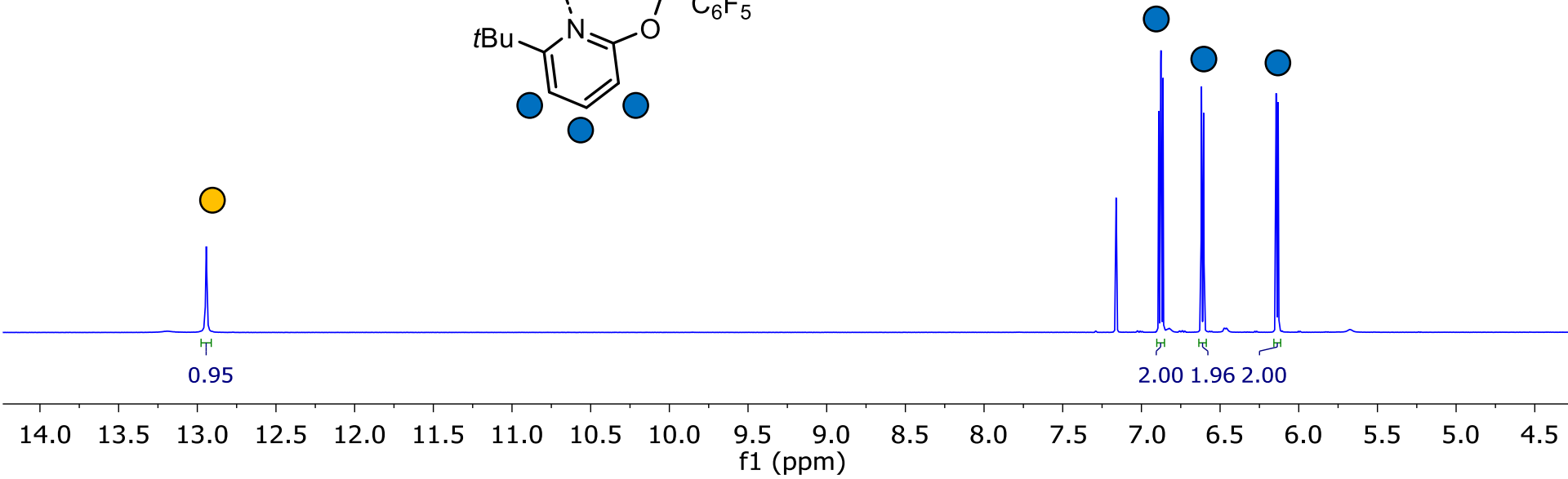

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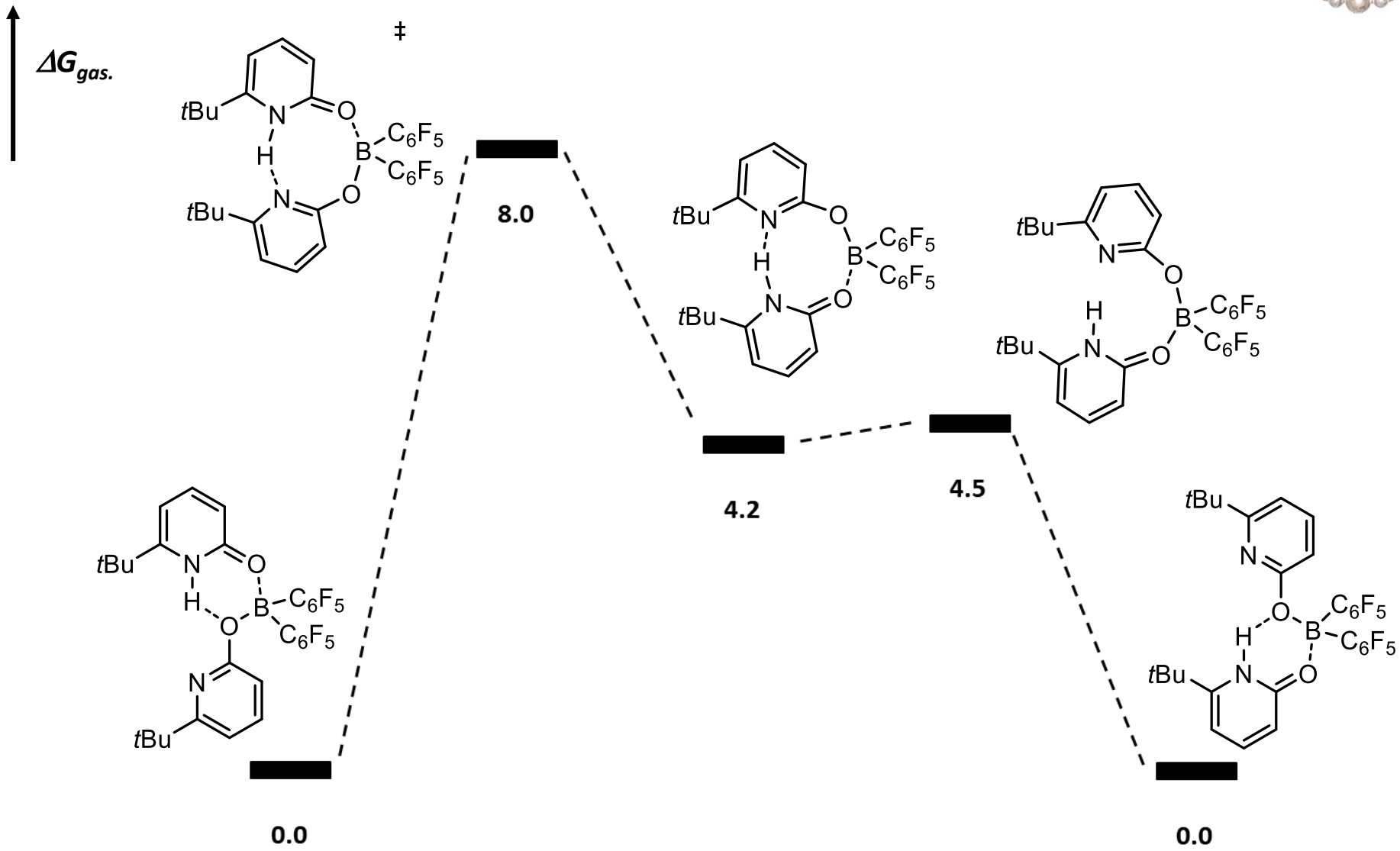
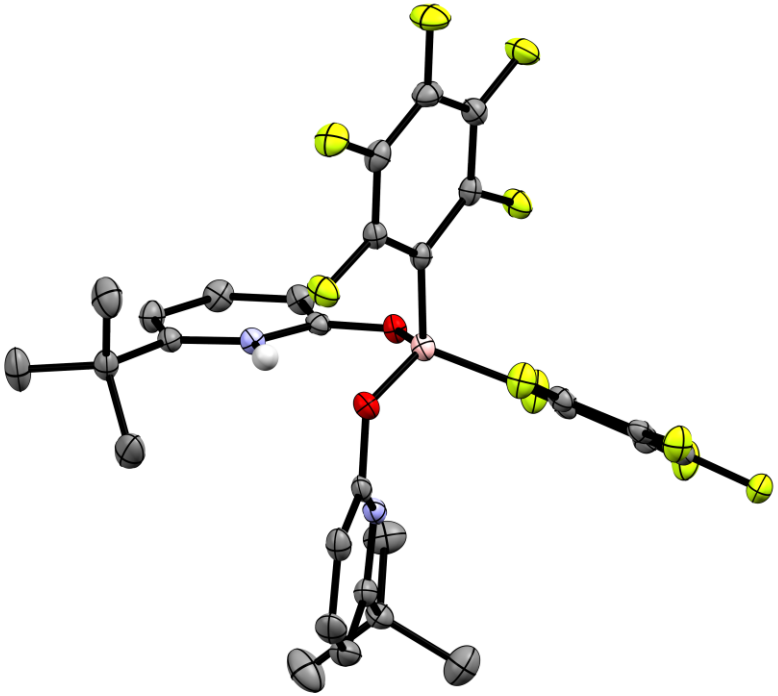
Deciphering the Reaction II

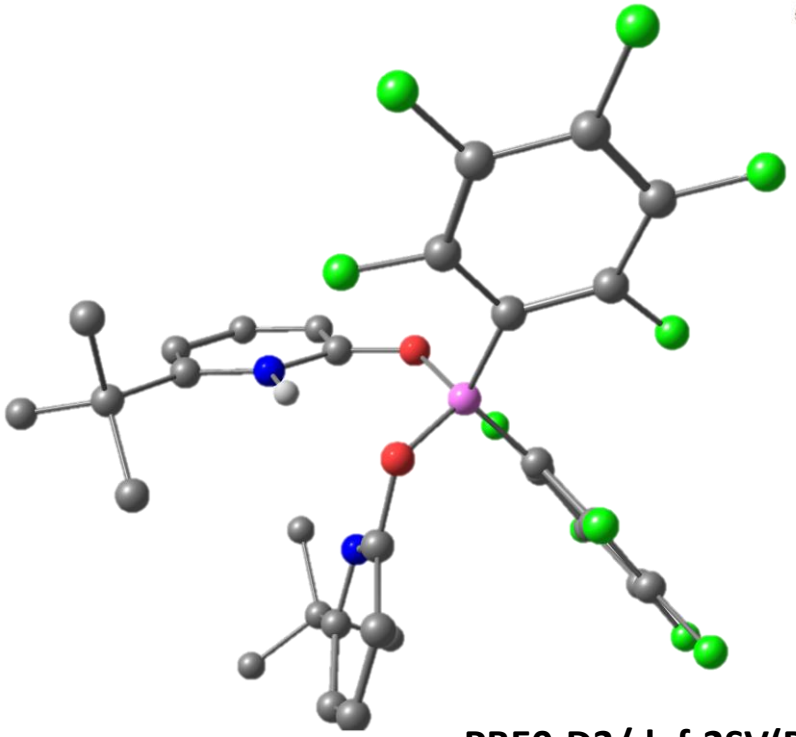


DLPNO-CCSD(T)/def2-TZVP//PBE0-D3/def2-SV(P)

Deciphering the Reaction II



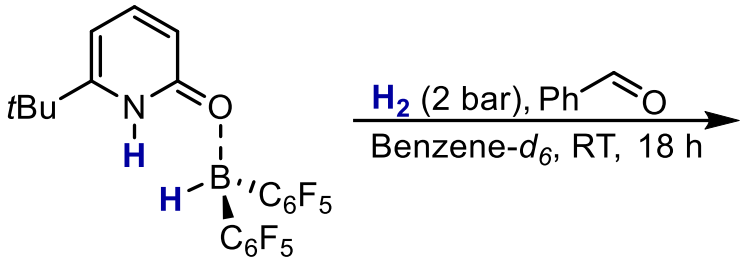
XRD-Structure

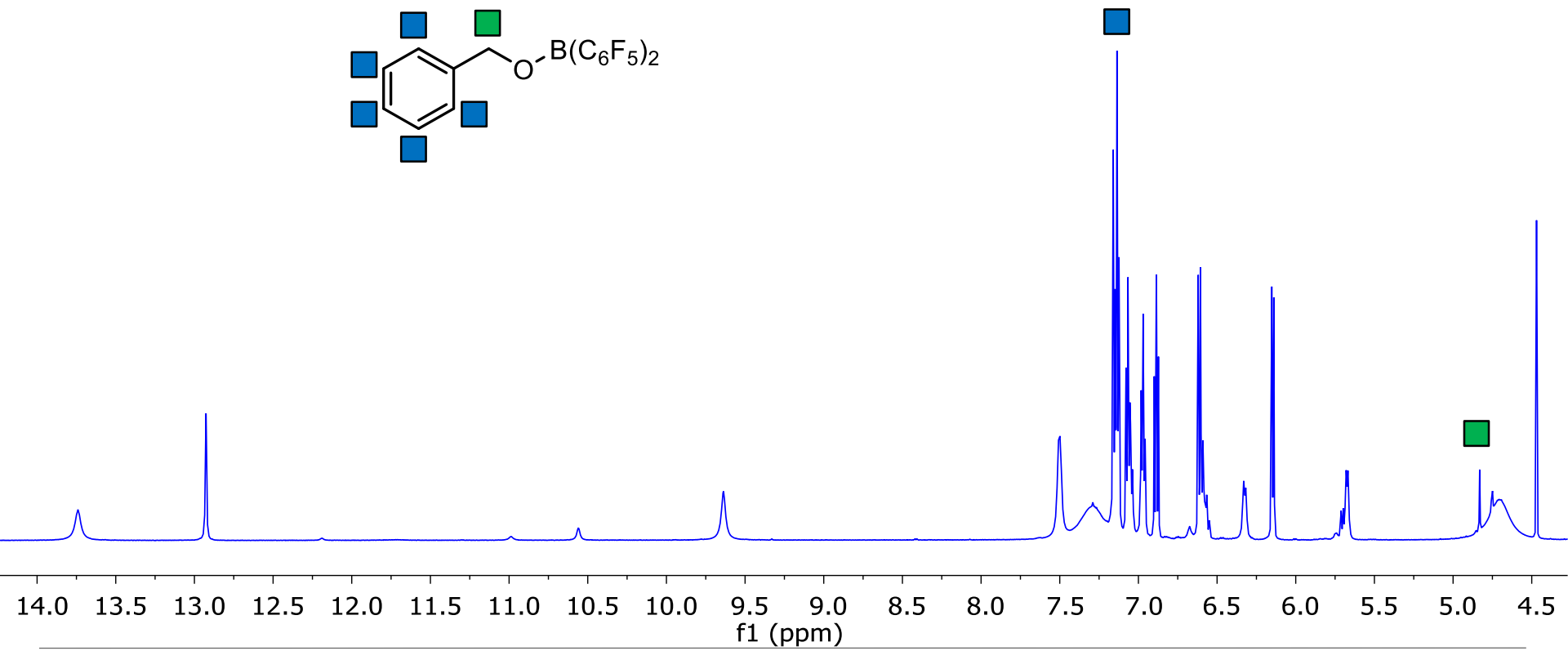


PBE0-D3/def-2SV(P)

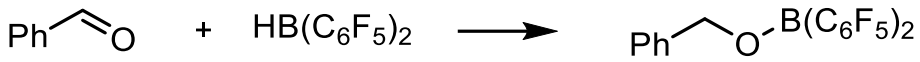
d / Å	XRD	DFT
$N^{6} – O^{20}$	2.700	2.701
$B^{22} \cdots O^{21}$	1.521	1.530
$B^{22} – O^{20}$	1.474	1.484
$C^{1} – O^{21}$	1.289	1.272

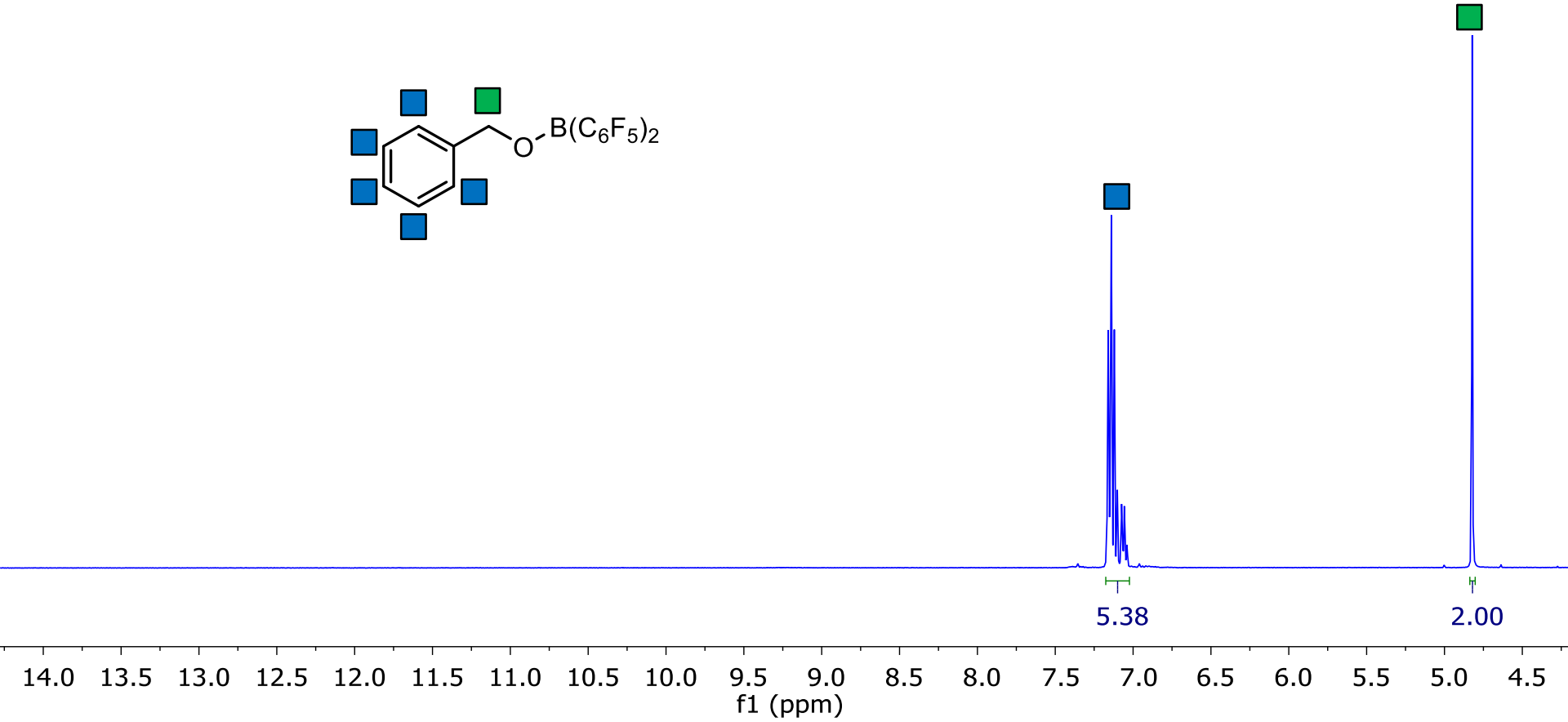
Deciphering the Reaction III





Deciphering the Reaction III





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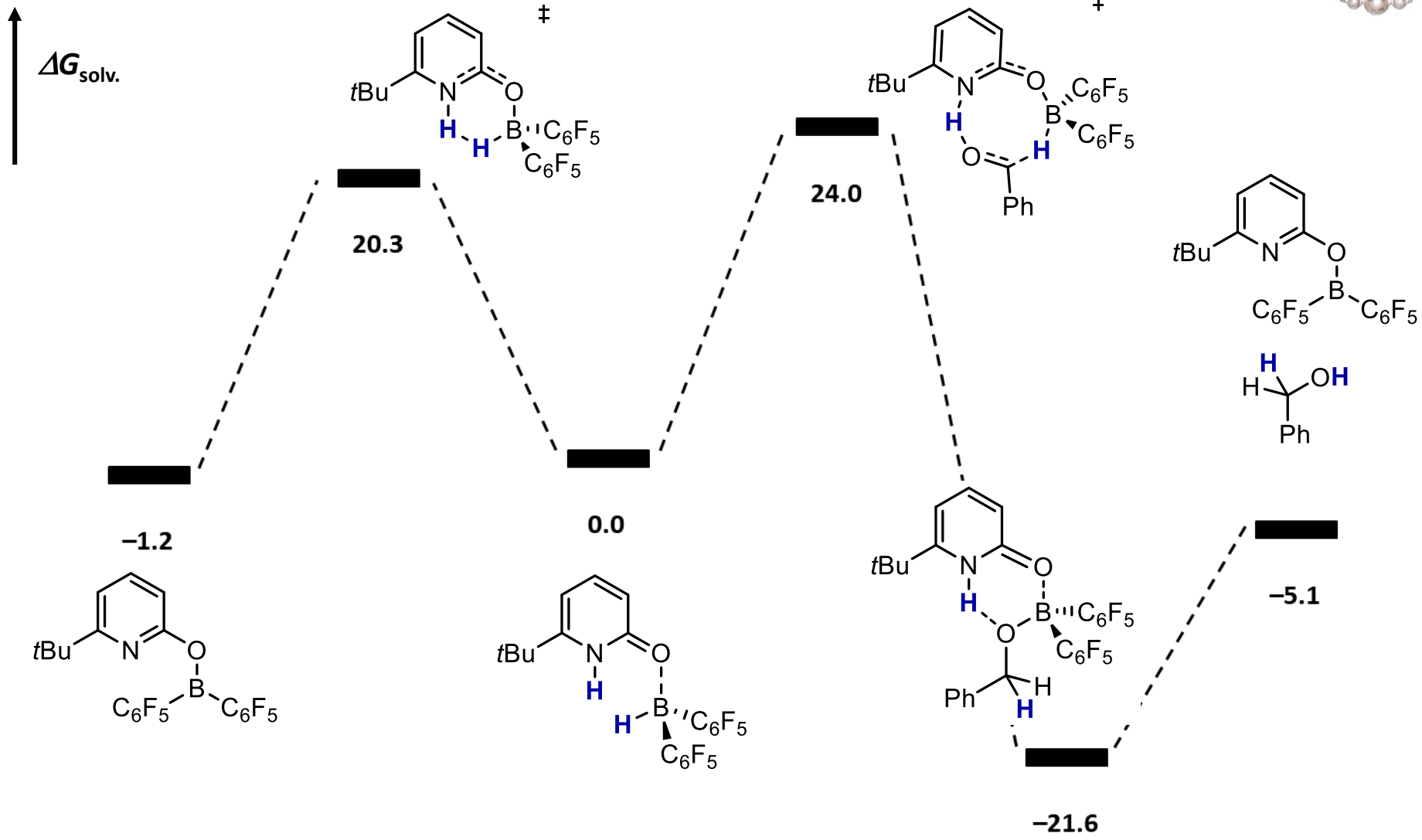
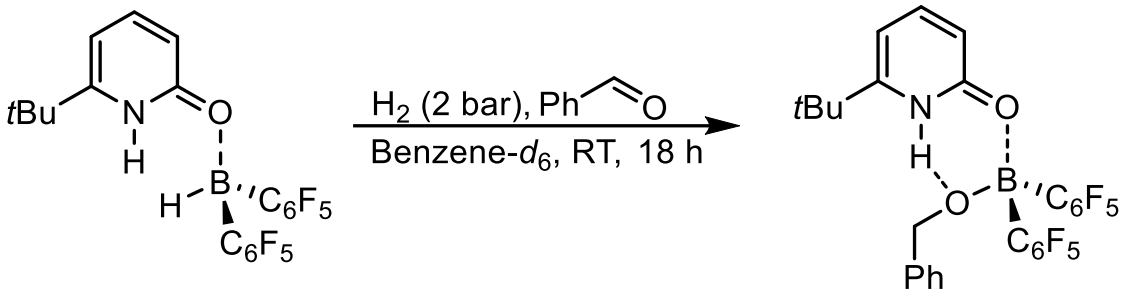
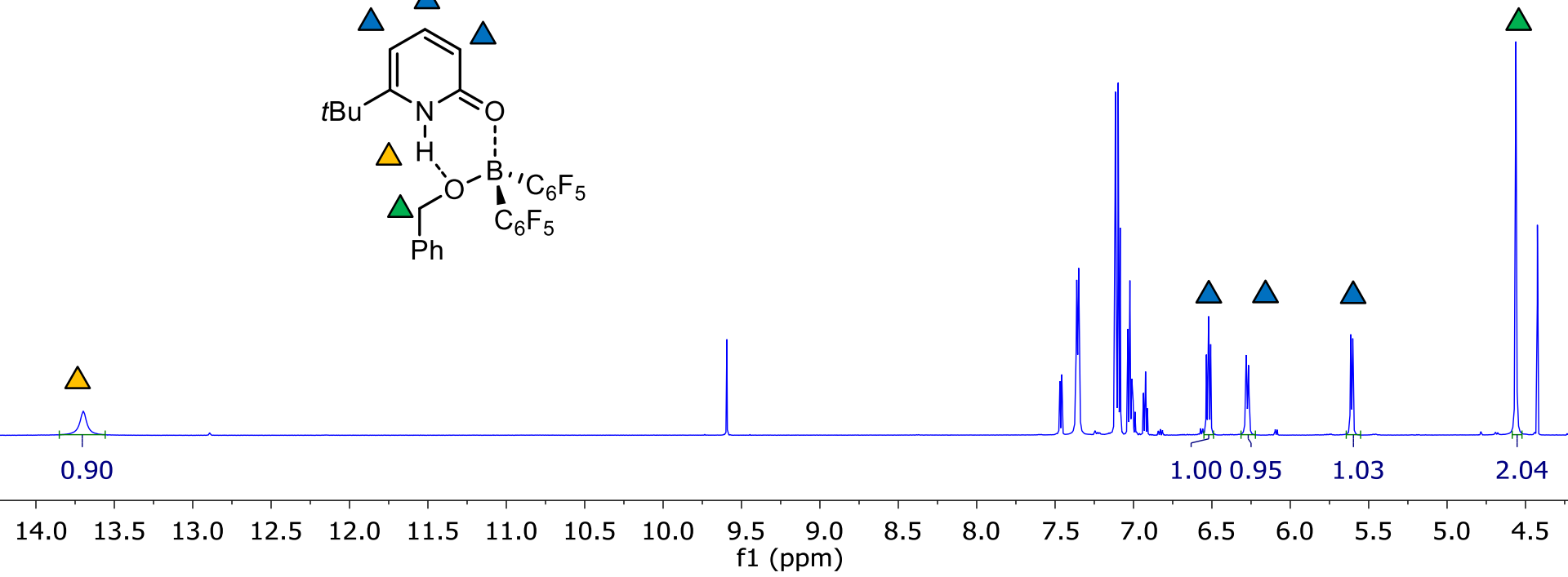
Reduction of Benzaldehyde: PES revised



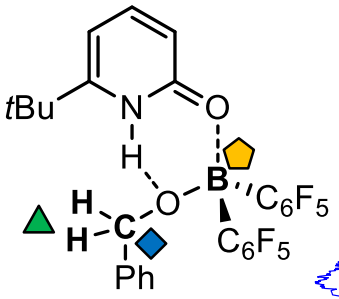
DLPNO-CCSD(T)/def2-TZVP//PBE0-D3/def2-SV(P)
SMD: Benzene

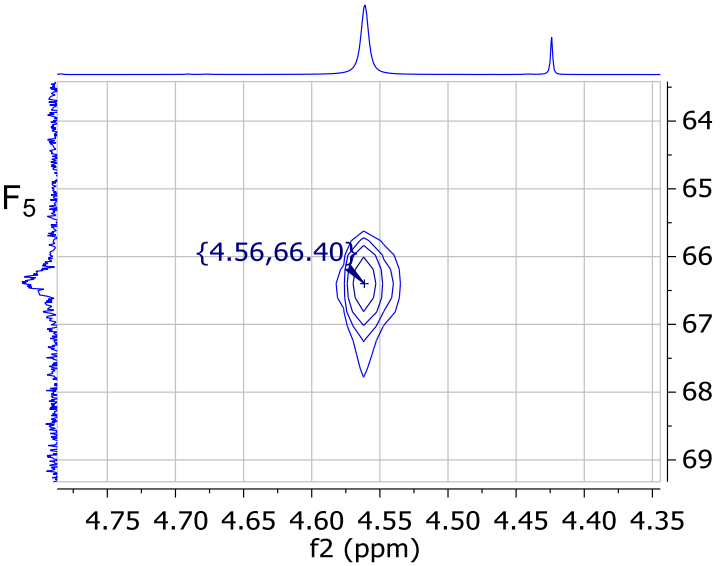
Reduction of Benzaldehyde: Reaction revised

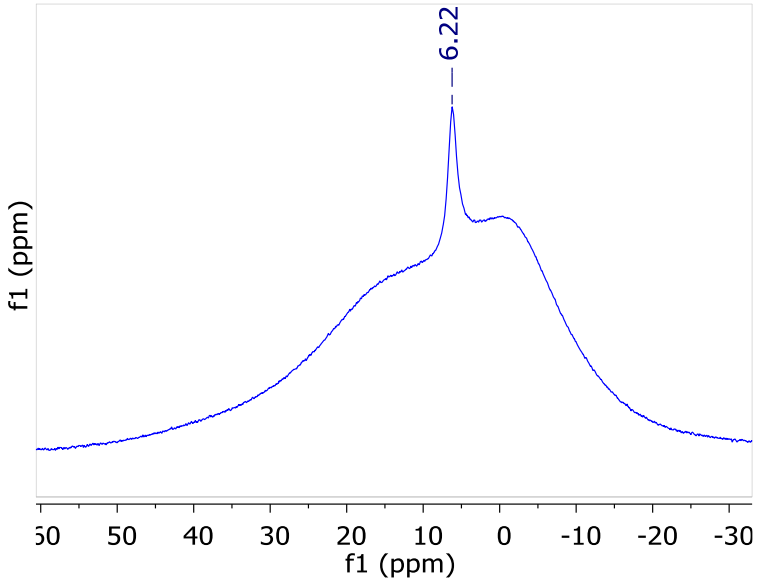




Reduction of Benzaldehyde: Reaction revised



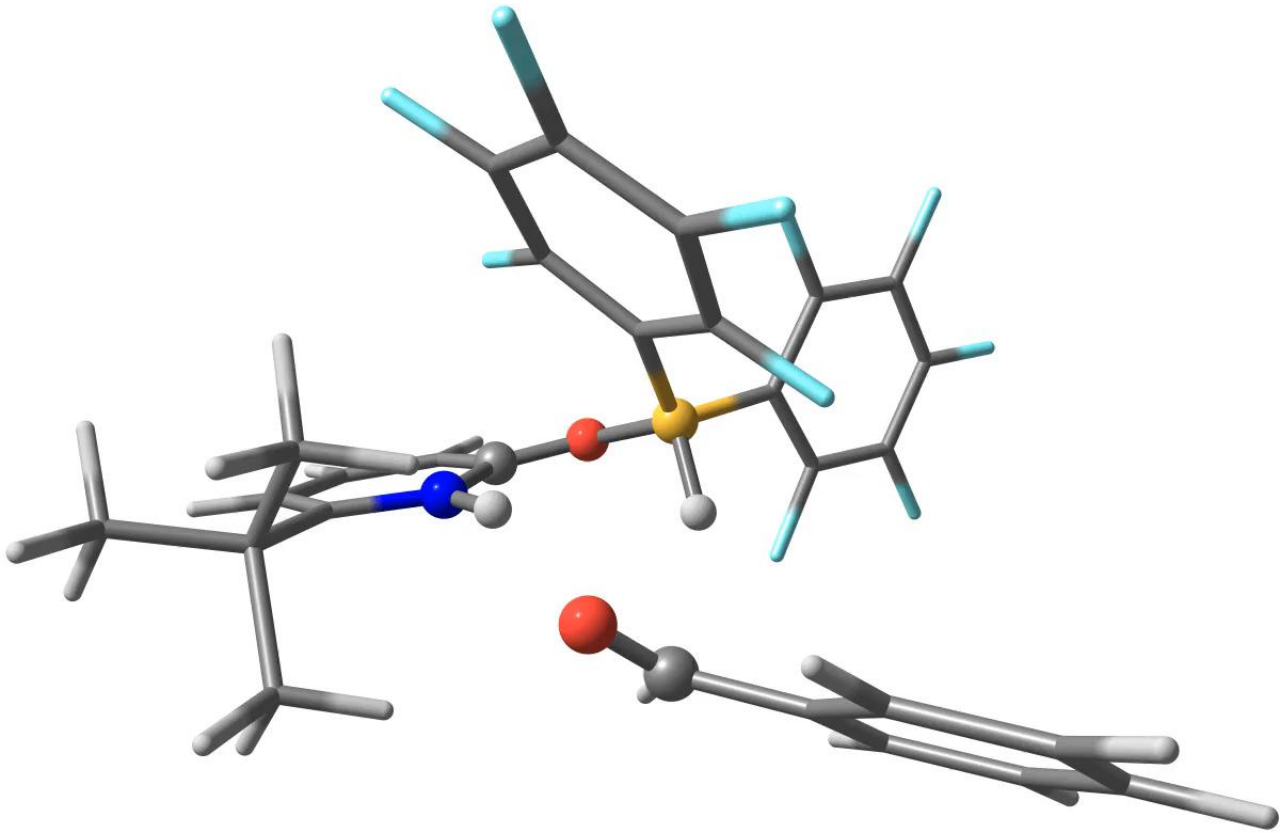




		δ / ppm (exp.)	δ / ppm (DFT)
▲	^{11}B	6.2	6.3
◆	^{1}H	4.56	4.76
⬟	^{13}C	66.4	68.7

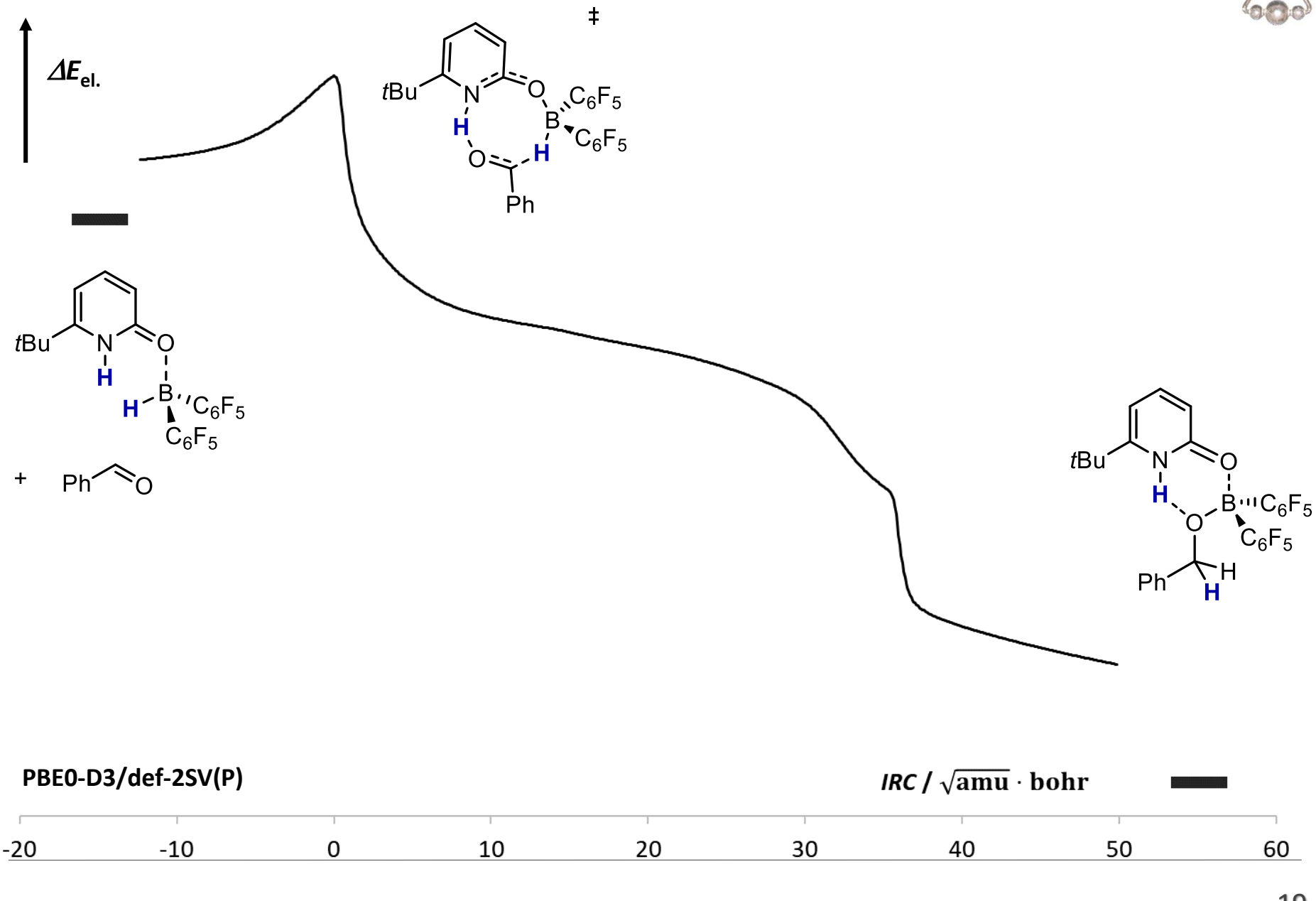
PBE0-D3/ def2-TZVP

Reduction of Benzaldehyde: Transition State

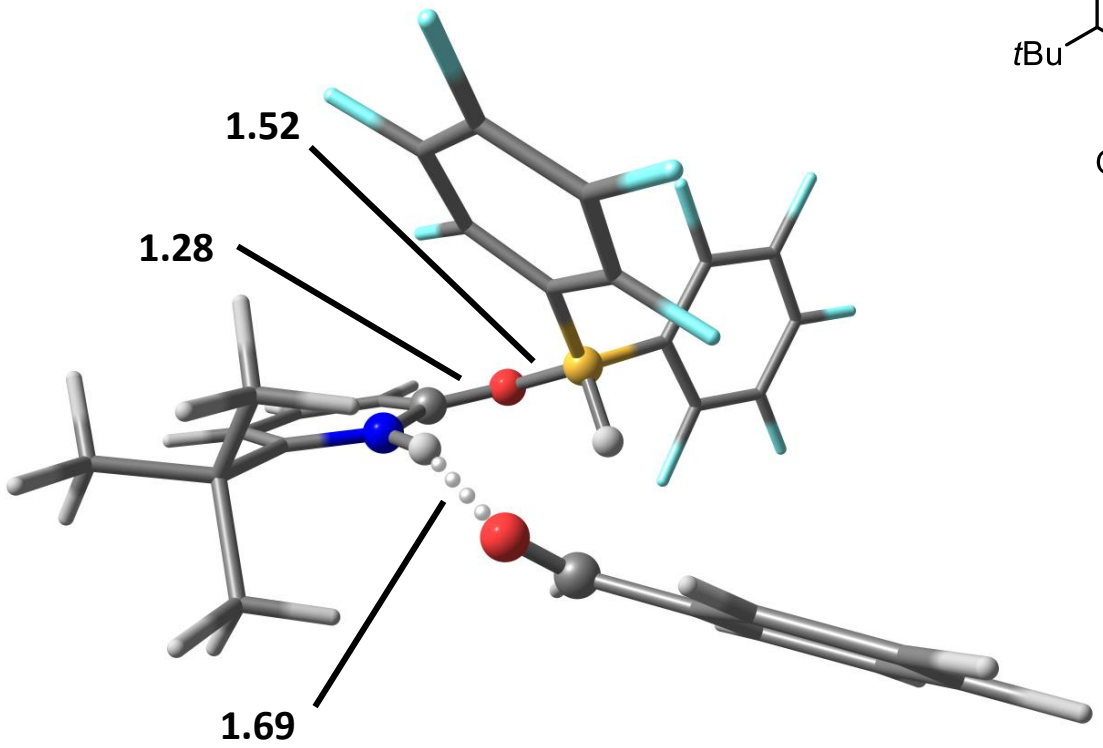


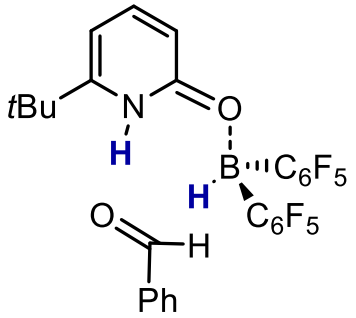
PBE0-D3/def-2SV(P)

Reduction of Benzaldehyde: Transition State: IRC



Reduction of Benzaldehyde: Transition State: IRC





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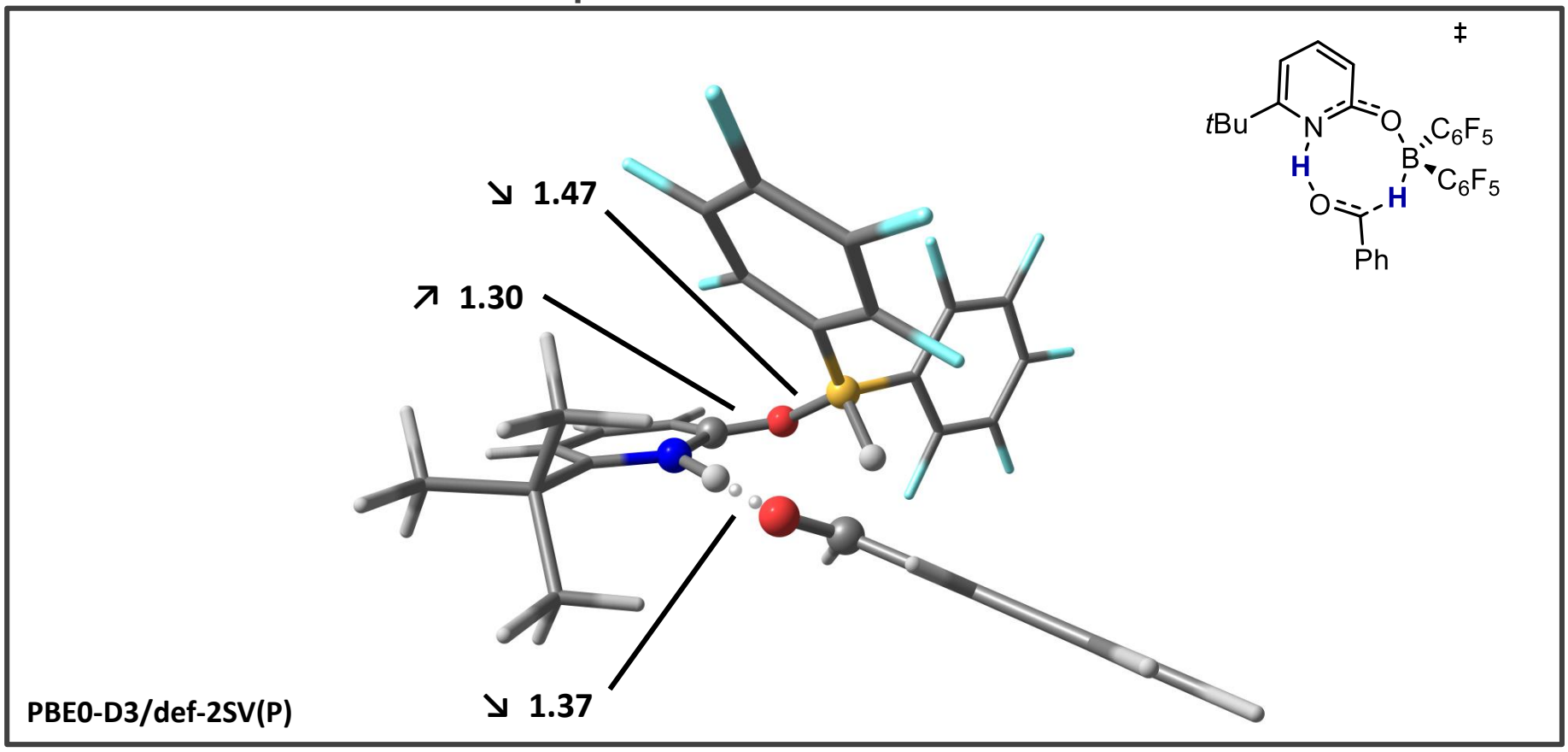
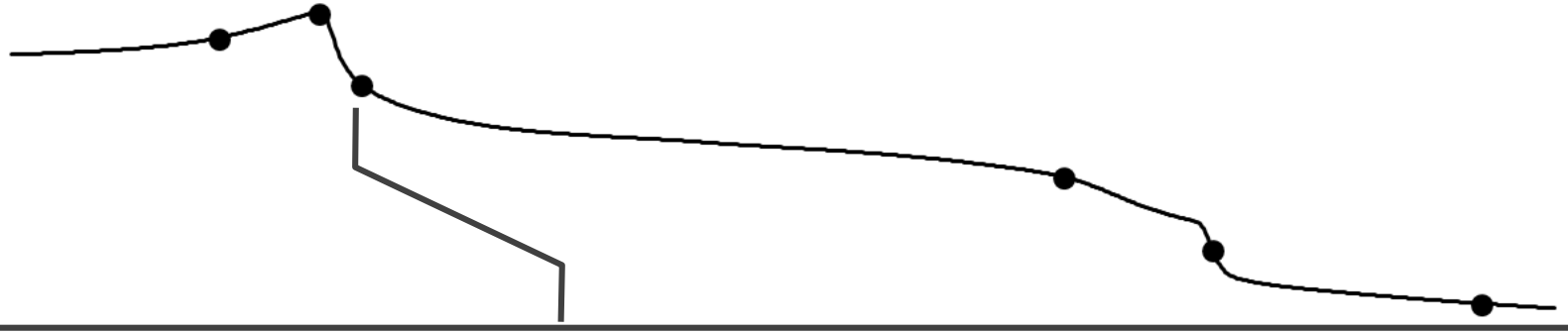
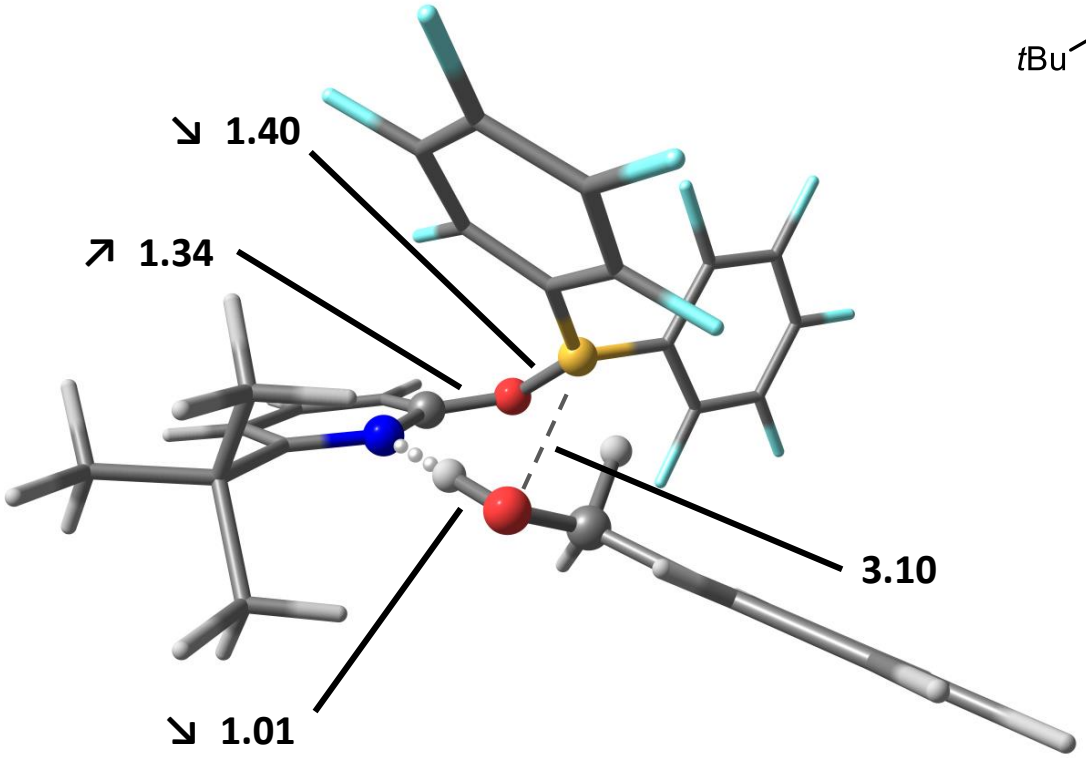
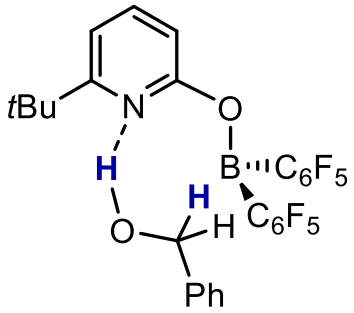
Reduction of Benzaldehyde: Transition State: IRC



Reduction of Benzaldehyde: Transition State: IRC

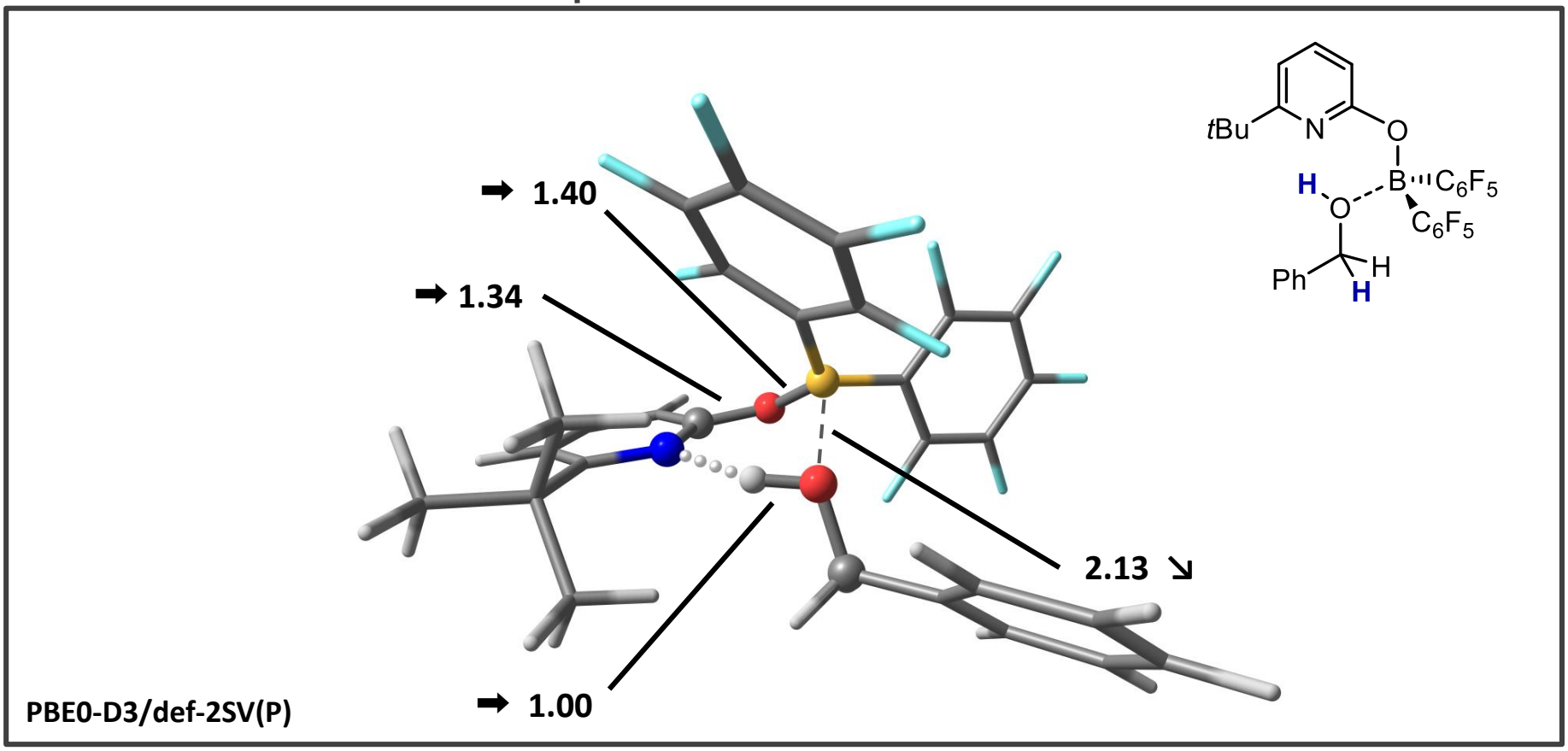




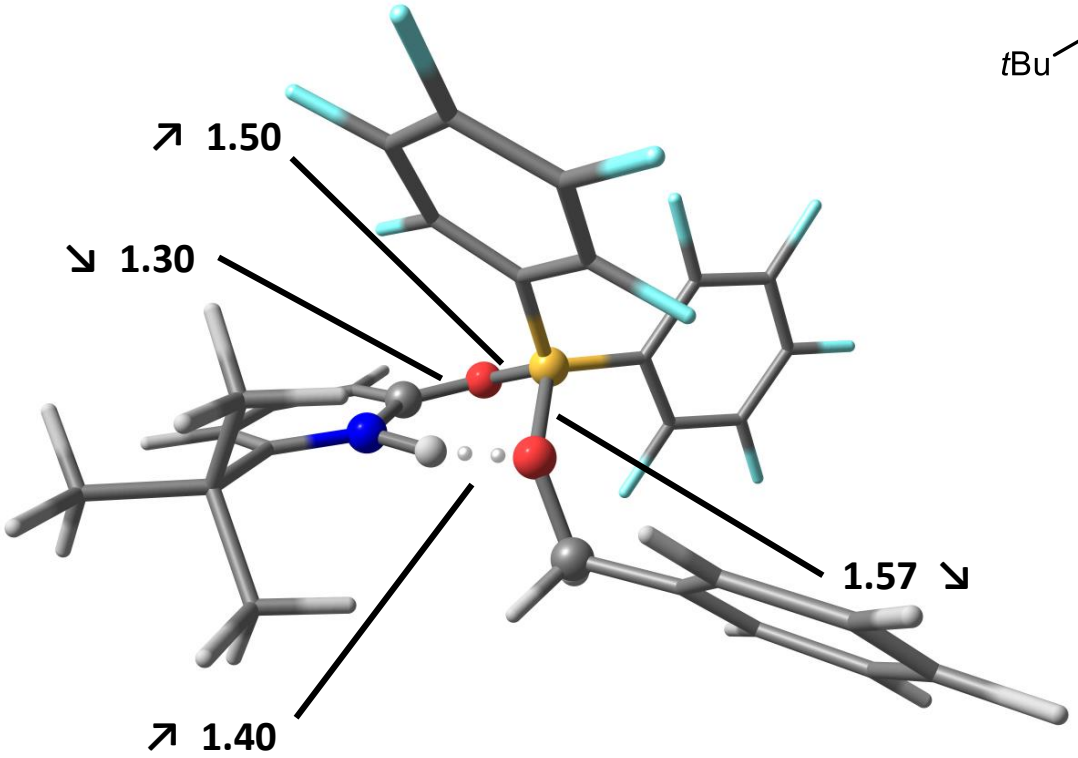


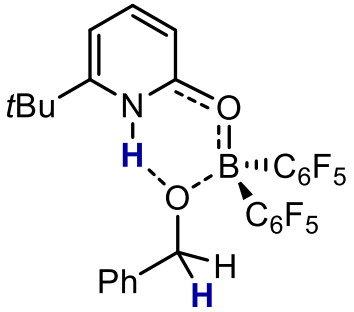
PBE0-D3/def-2SV(P)

Reduction of Benzaldehyde: Transition State: IRC



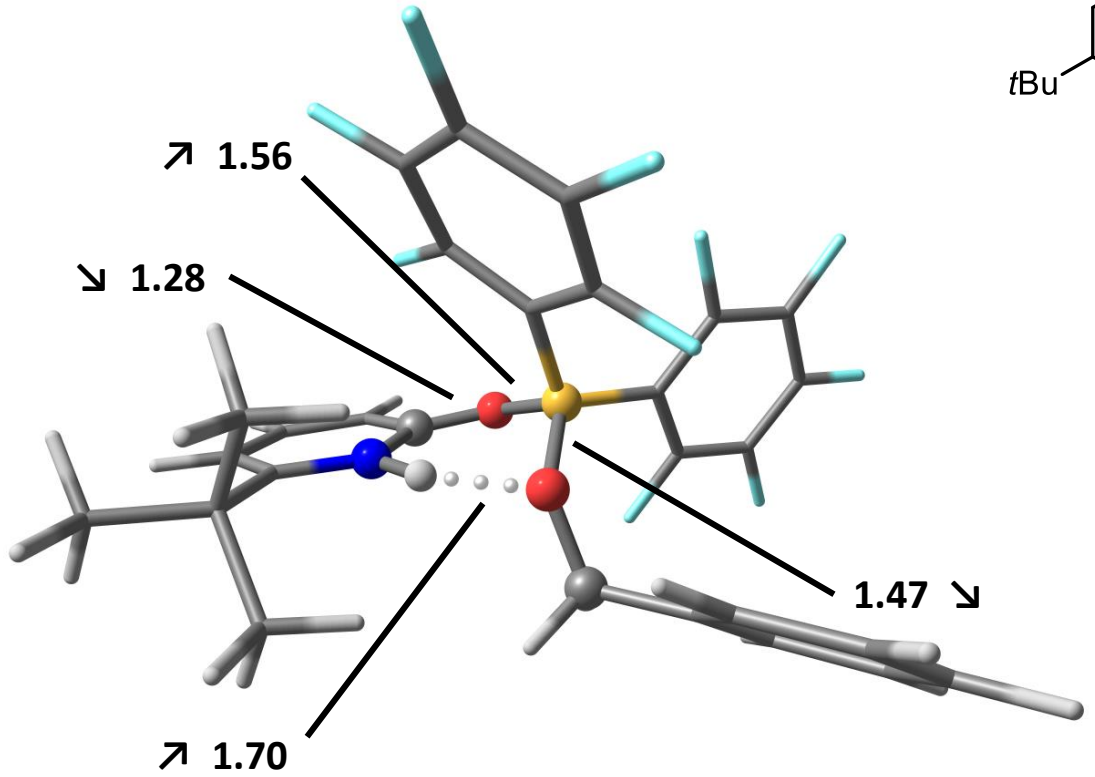
Reduction of Benzaldehyde: Transition State: IRC

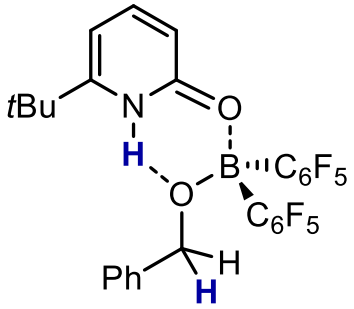




PBE0-D3/def-2SV(P)

Reduction of Benzaldehyde: Transition State: IRC





PBE0-D3/def-2SV(P)

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- Prof. Dr. Wegner and group
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