UNDERSTANDING SUZUKI-MIYAURA (SM) REACTION VIA WEBMO CALCULATIONS

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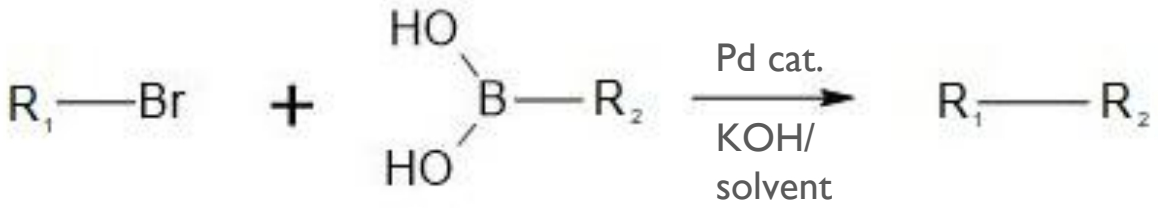
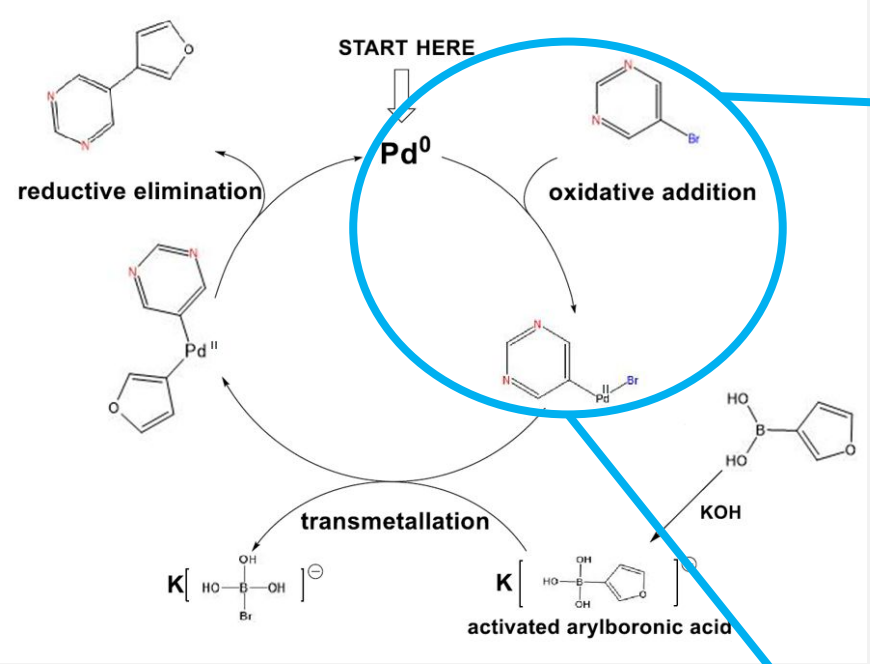
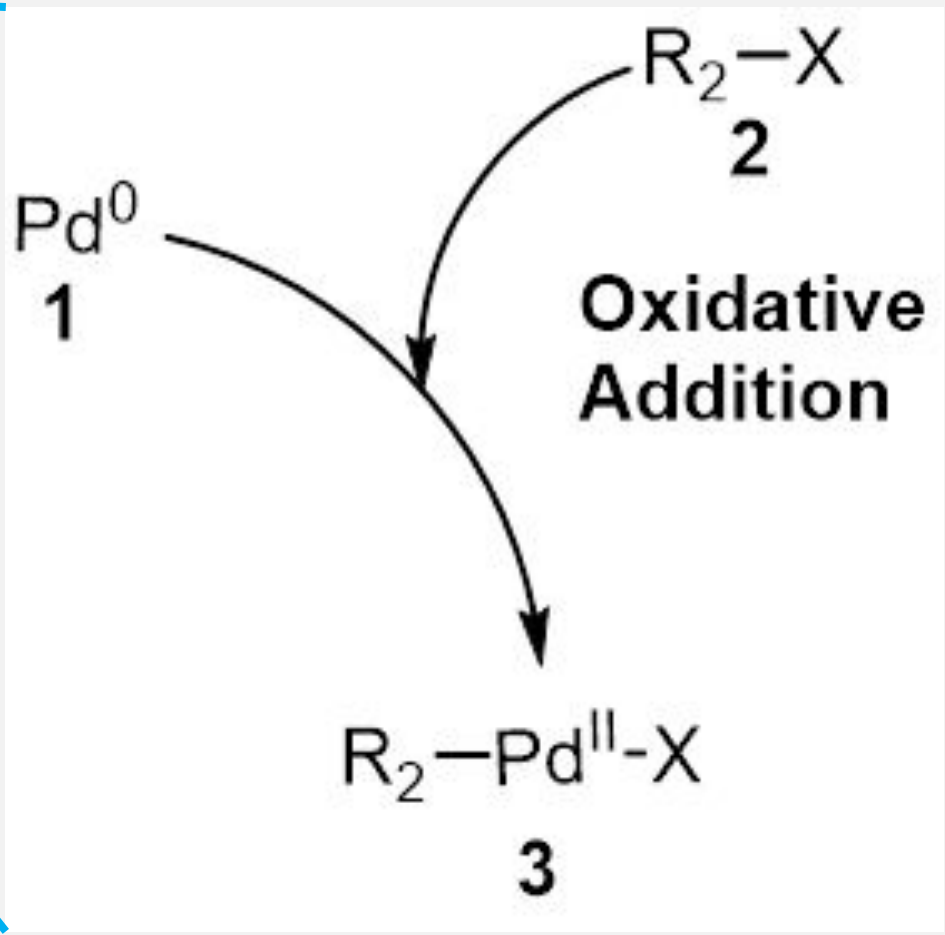
THE SUZUKI-MIYAURA REACTION (SM)

- SM coupling is a metal-catalyzed carbon-carbon bond reaction between organoboron and organohalide under basic conditions
  - Cross-coupling reactions are typically catalyzed by the expensive palladium (Pd) catalyst.
  - Commonly used in pharmaceuticals, polymers, and agrochemicals.



MECHANISM


START HERE
Pd0
oxidative addition
reductive elimination
Pd II
transmetallation
KOH
activated arylboronic acid


R2—X
2
Pd0
1
Oxidative
Addition
R2—PdII-X
3

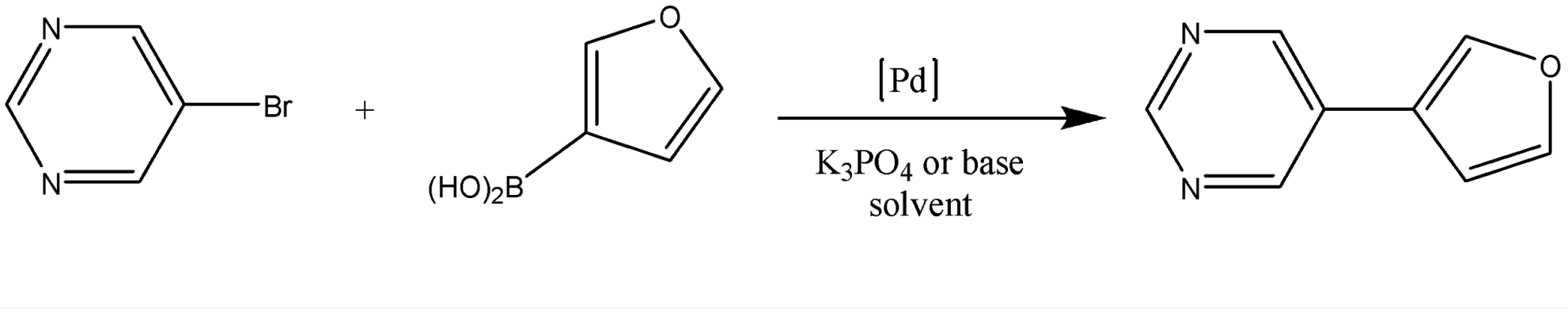
GAPS IN KNOWLEDGE

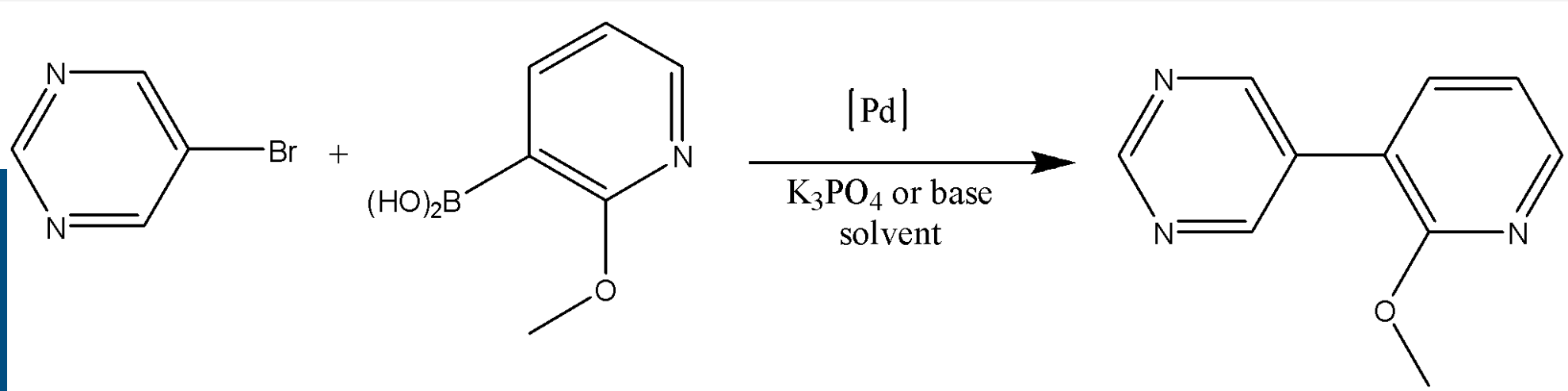
- Most studies have focused on trying different reactants, optimizing reaction conditions, and investigating different metal catalysts
- Limited studies focus on the individual mechanistic steps
- Using WebMO to obtain properties of reactants and product of SM reaction

OBJECTIVES

- Study chemical properties of reactants and products
  - ΔH reaction value
  - Bond dissociation energy (BDE)
- Characterize products by
  - IR
  - NMR
  - UV-Vis
- Determine the factor(s) affecting the 1st step in the mechanism of SM reaction
  - Find best halogen for reaction (F, Cl, Br)

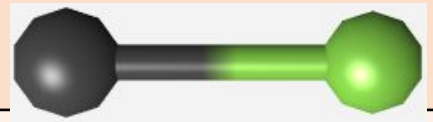
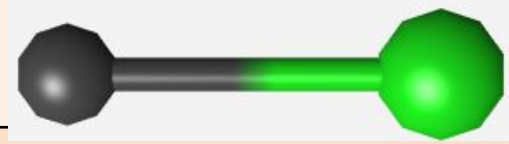
METHODOLOGY: SM REACTIONS EXAMINED





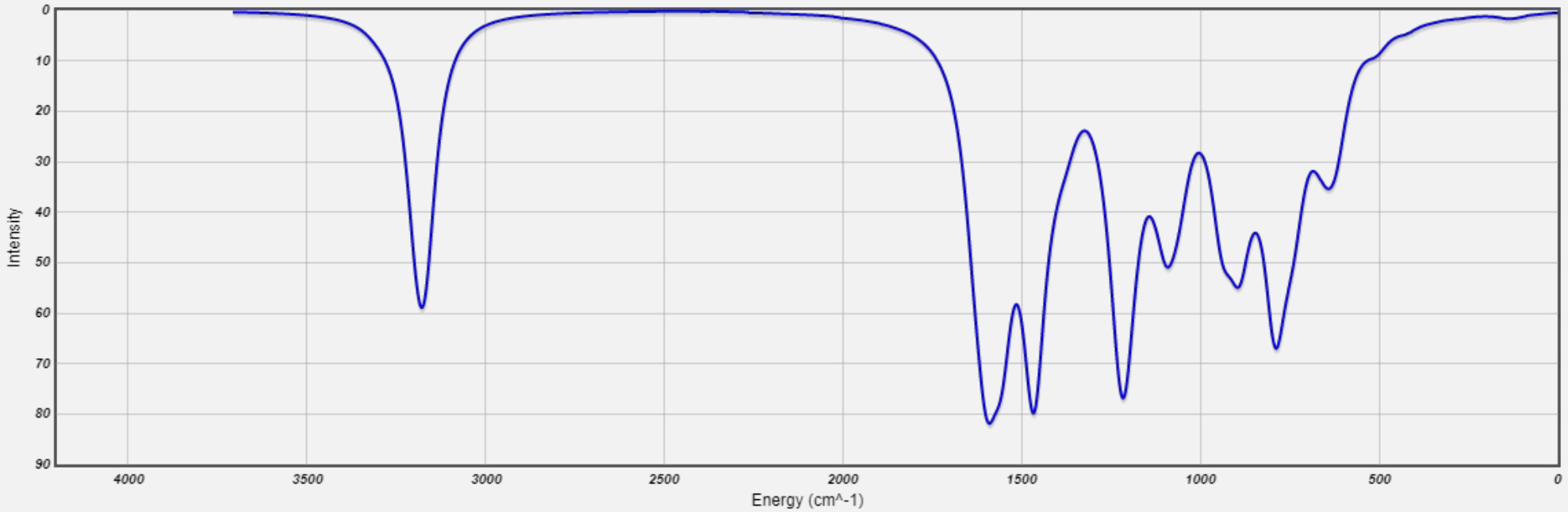
RESULTS
ΔH & BDE

- ΔH reaction value: $\Delta_r H$: [ΣH(product) - ΣH(reactants)](627.51kcal/mol^{-1})/ E_h)
  - Reaction 1: 1,724,589.30325 kcal/mol or 1.725×10^6 kcal/mol
  - Reaction 2: 1,724,592.19502 kcal/mol or 1.725×10^6 kcal/mol

Chemical Formula	3D Molecular Image	BDE	Å
CF		*127.255*	1.342
CCl		*91.459*	1.746
CBr		*84.086*	1.900

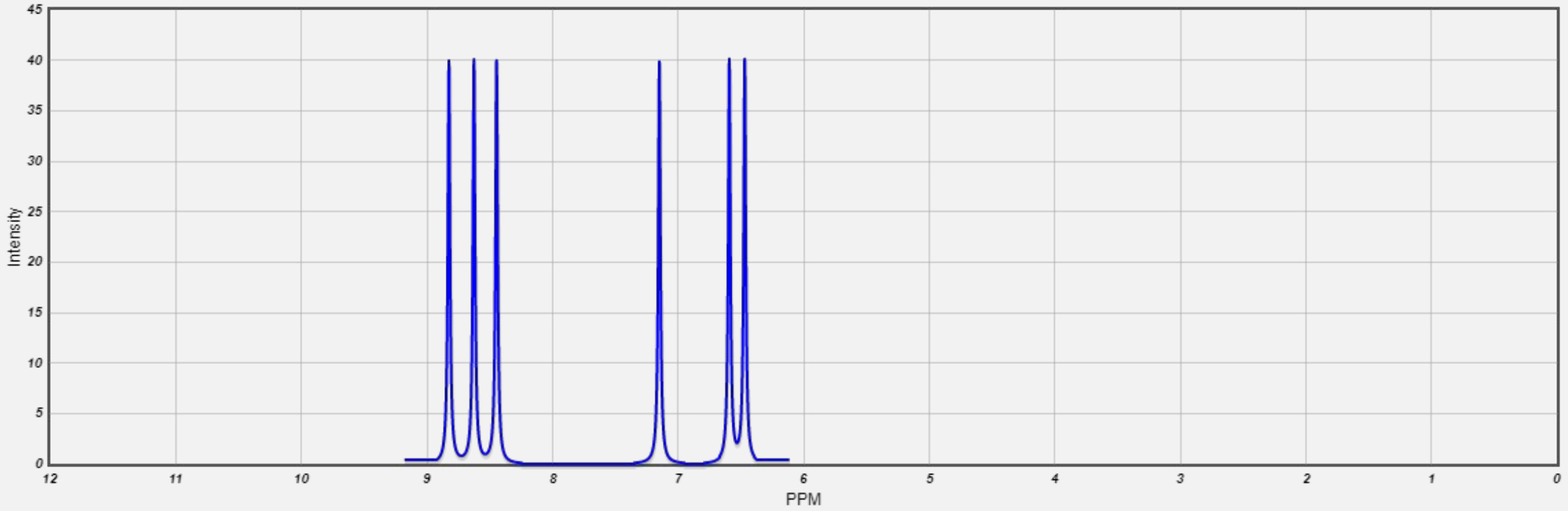
RESULTS
IR SPECTRUM (PRODUCT 1)

5-(furan-3-yl)pyrimidine



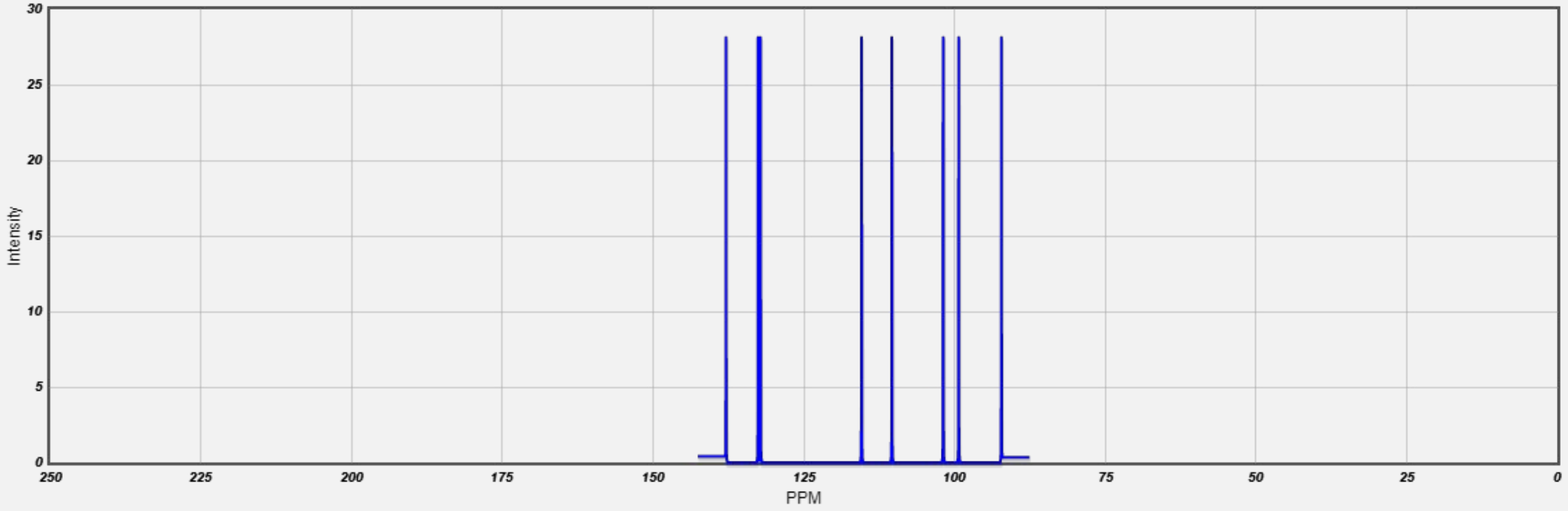
RESULTS
^{1}H NMR OF (PRODUCT 1)

5-(furan-3-yl)pyrimidine



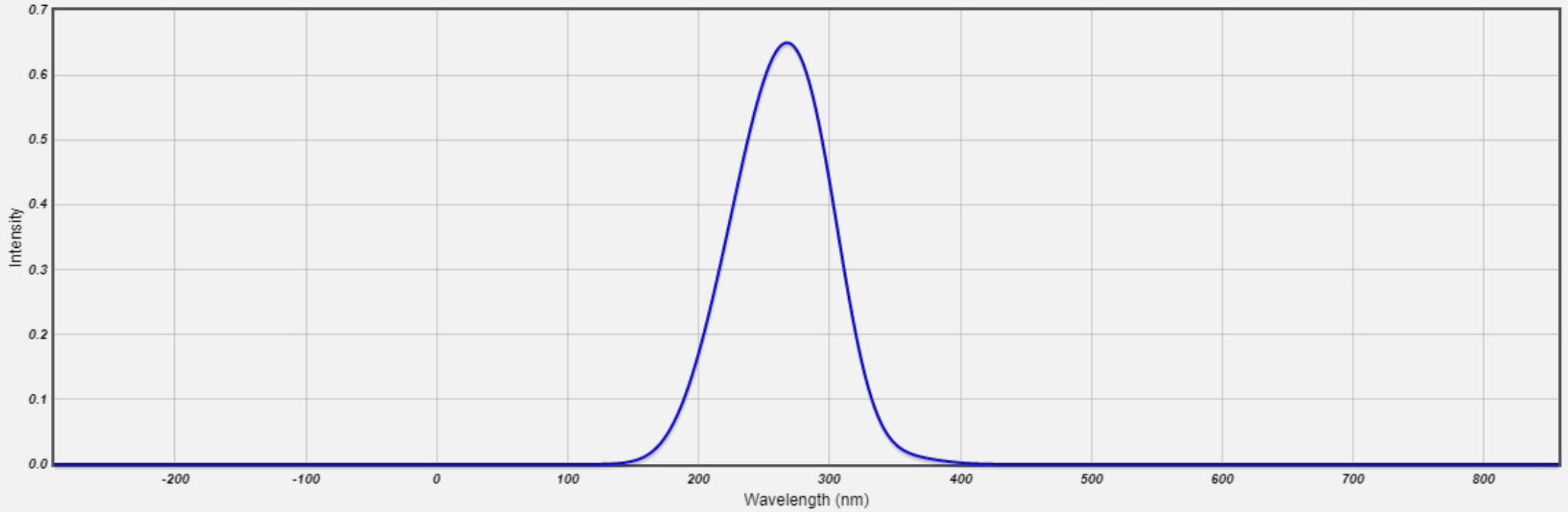
RESULTS
^{13}C NMR (PRODUCT 1)

5-(furan-3-yl)pyrimidine

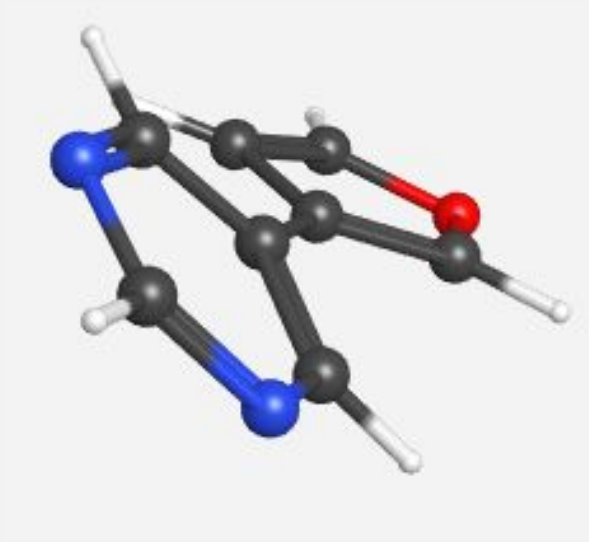


RESULTS
UV-VIS (PRODUCT 1)

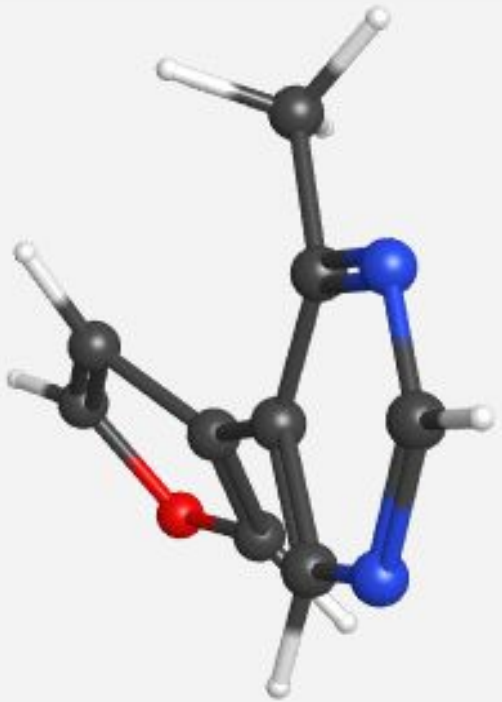
5-(furan-3-yl)pyrimidine



RESULTS
DIHEDRAL ANGLES (PRODUCT 1)



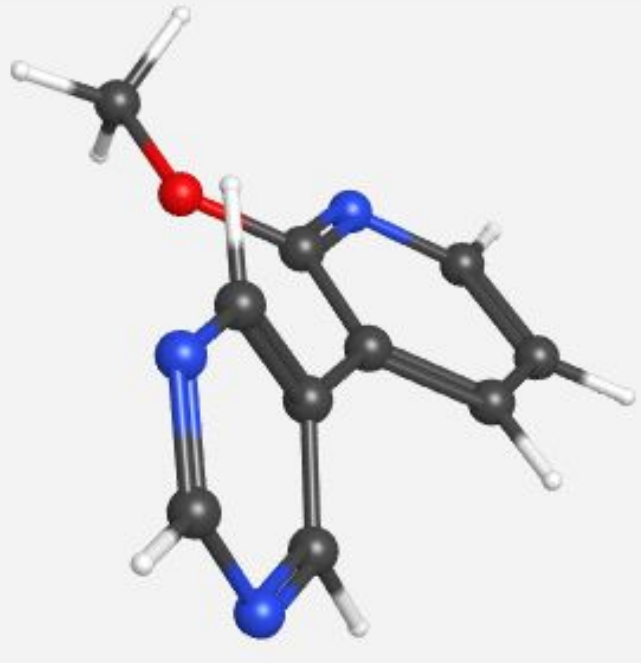
26.309°



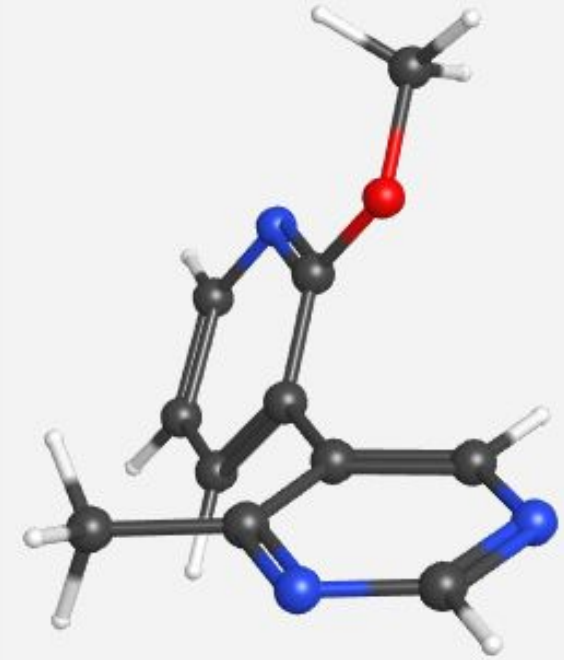
41.659°

80.586°

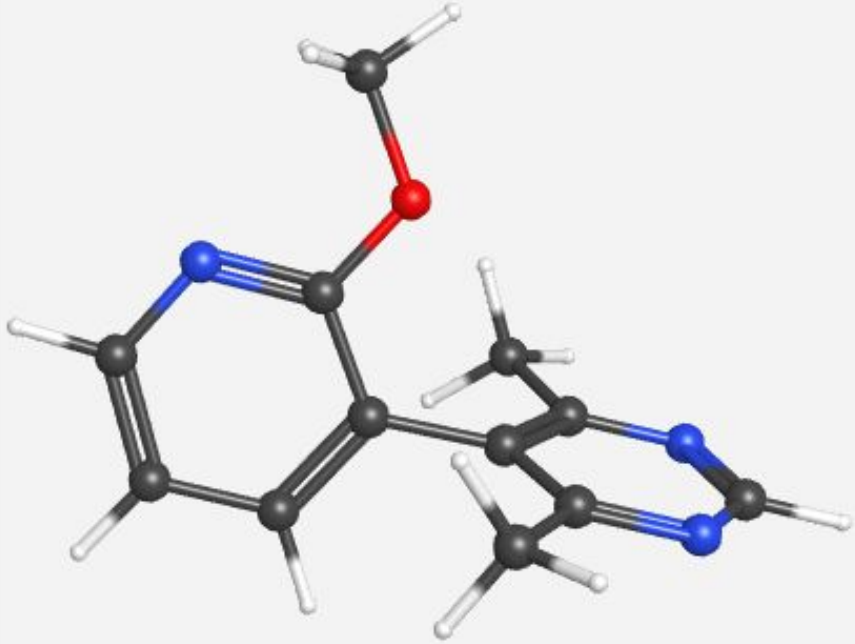
RESULTS
DIHEDRAL ANGLES (PRODUCT 2)



39.543°



56.765°



74.815°

CONCLUSION

- Chemical properties were successfully obtained using WebMO
- Characterization can be done by WebMO calculations - a great way to confirm product's properties for newer reactant combinations
- The C-Br bond is more reactive toward oxidative addition than the C-F bond due to the small BDE value of organobromide and thus the coupling product will form via the C-Br bond.
- The molecule changes from flat to 3D shape once substituents are added to the phenyl ring

FUTURE WORK

- In our research we observed the determining the factor(s) affecting the 1st step in the mechanism of SM reaction.
- Future investigation of the proceeding steps in the mechanism of SM reactions is viable research to pursue

ACKNOWLEDGMENTS

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