Supporting Information for:

Mechanisms and Reactivity of Tl(III) Main-Group Metal-Alkyl Functionalization in Water

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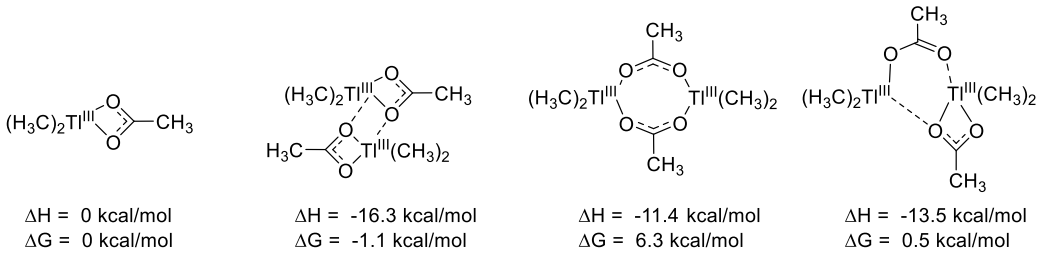
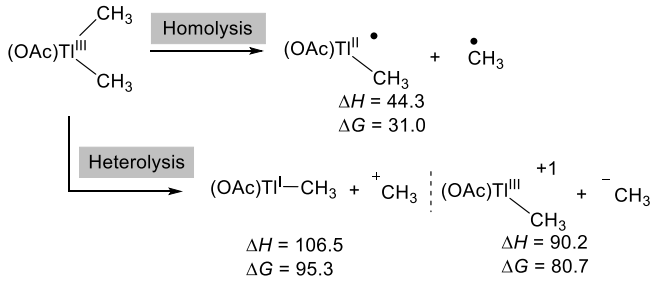
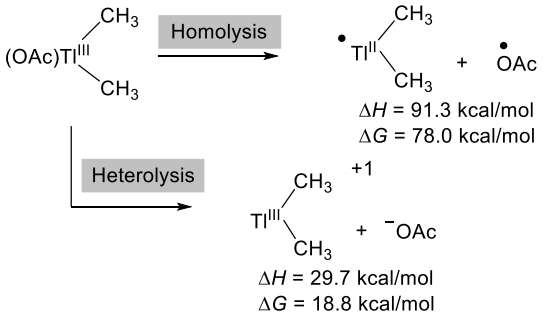


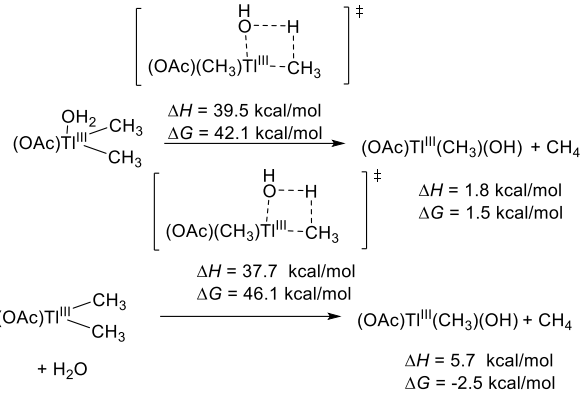
2. Scheme S2. Bond dissociation energies for the Tl–C bond of $(OAc)Tl^{III}(CH_3)_2$.



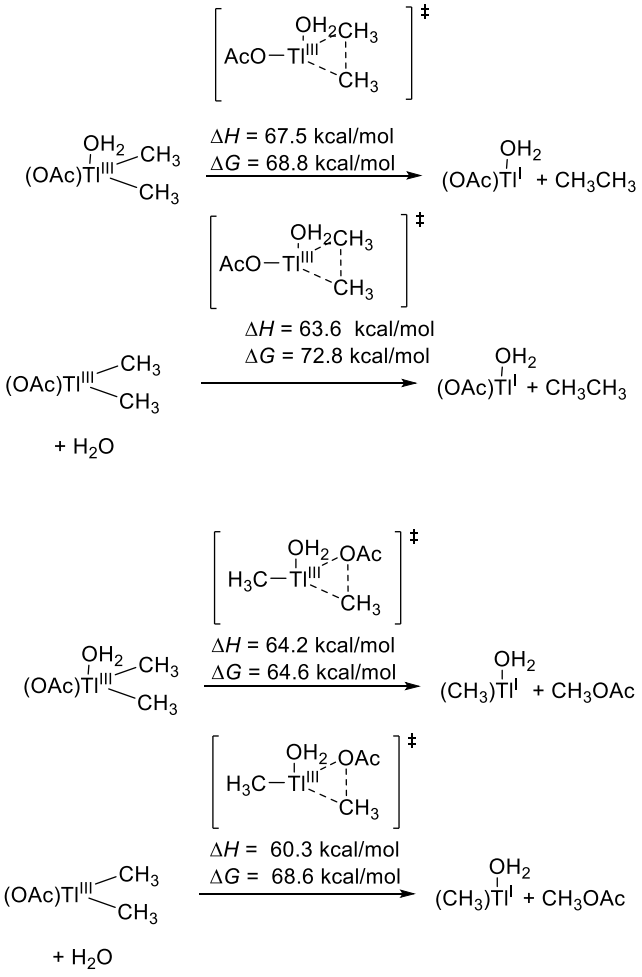
3. Scheme S3. Bond dissociation energies for the Tl–O bond of $(OAc)Tl^{III}(CH_3)_2$.



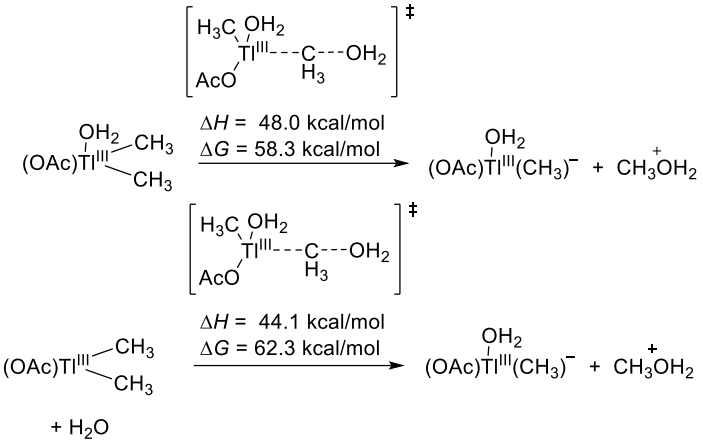
4. Scheme S4. Protonolysis

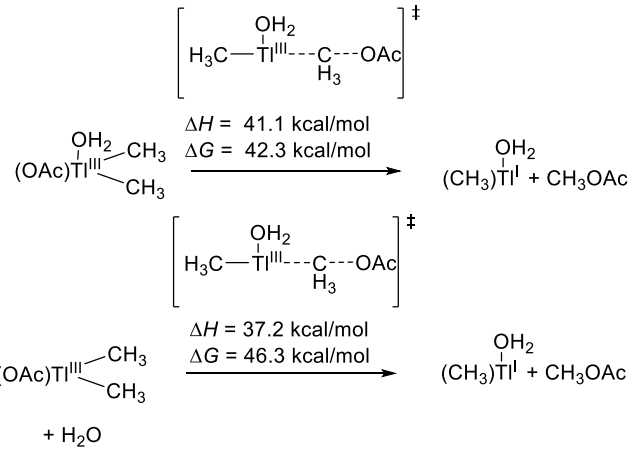


5. Scheme S5. Tl–dimethyl reductive elimination transition states with water.

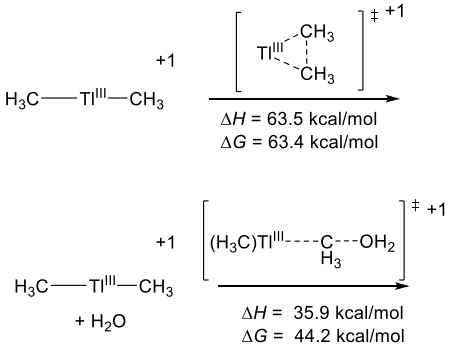


6. Scheme S6. Tl–dimethyl reductive substitution transition states with water.





7. Scheme S7. $Tl(CH_3)_2^+$ cation functionalization transition states.



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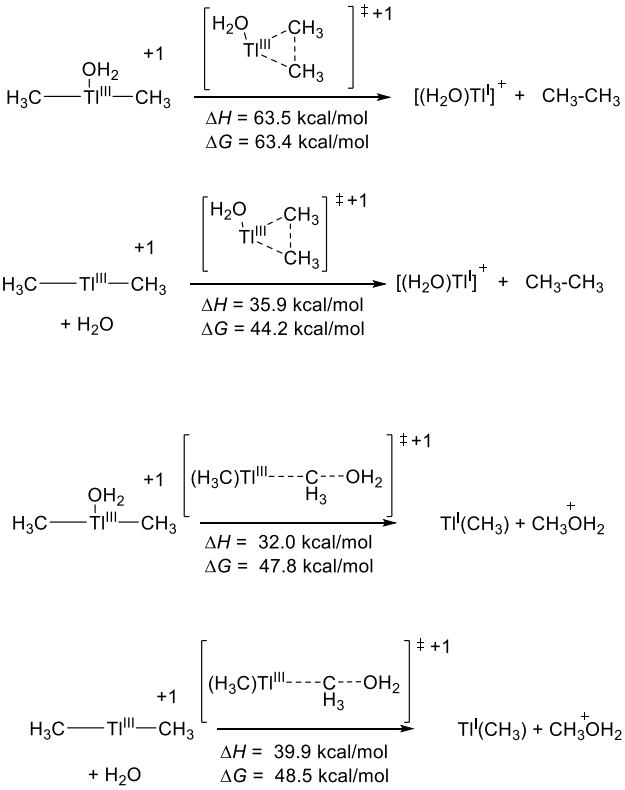

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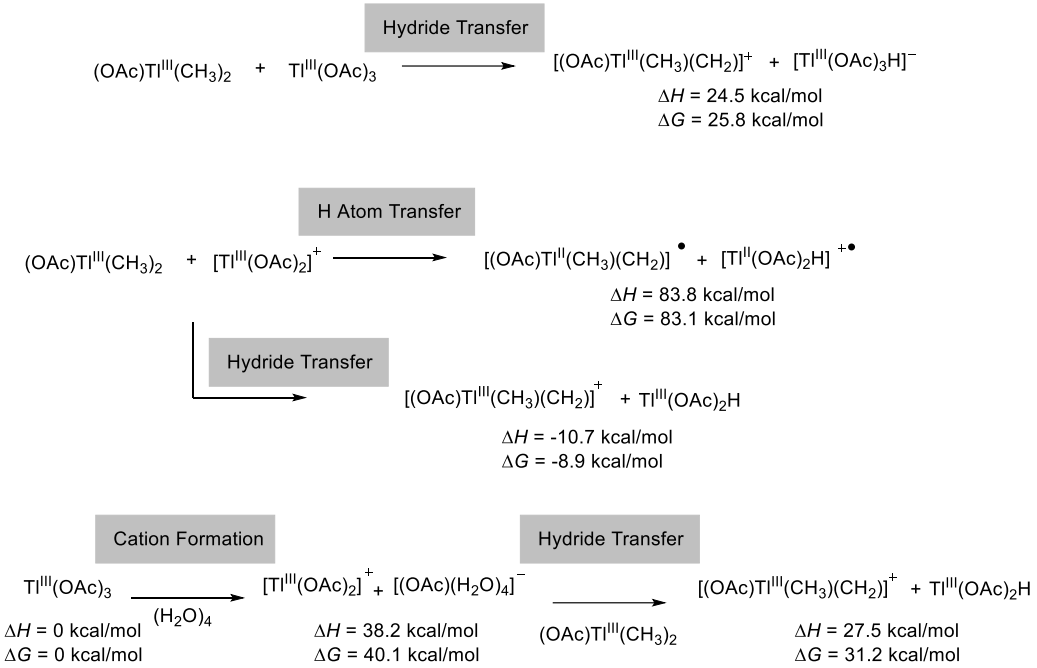
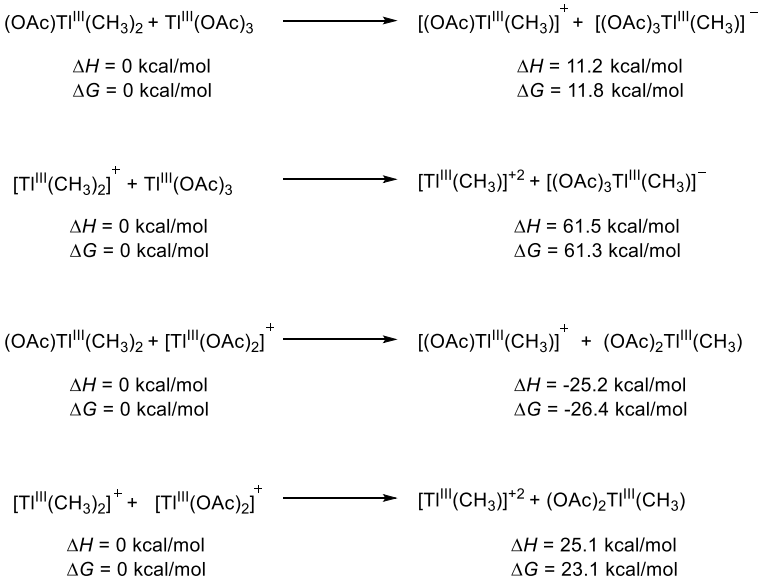


10. Scheme S10. Thermodynamics for methyl transfer.



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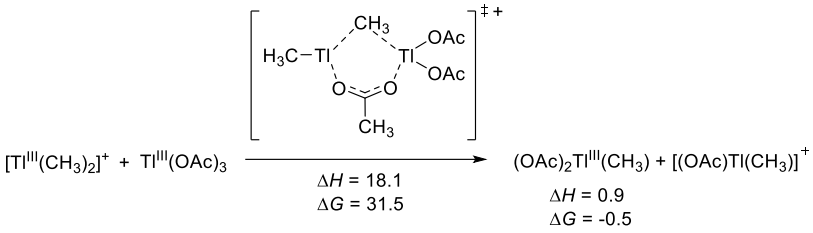

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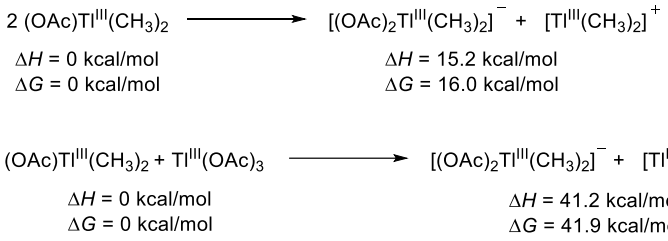

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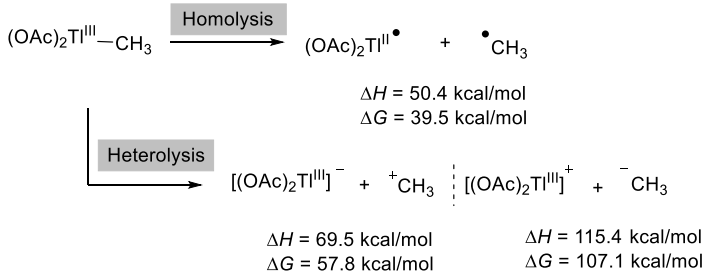

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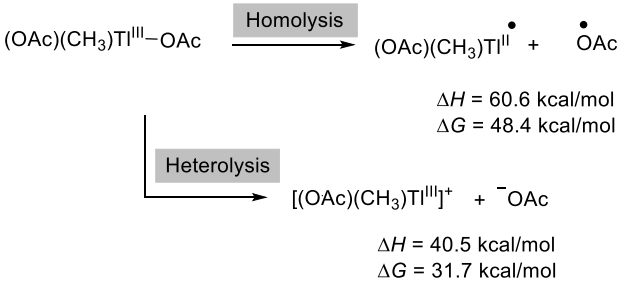

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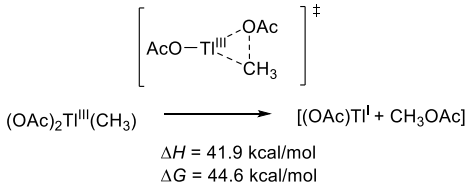

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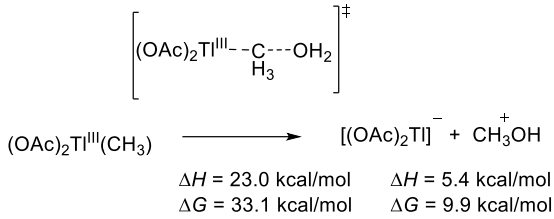

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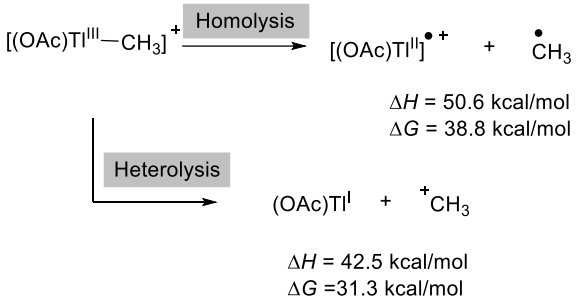

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