



Université de Montréal, Montréal, QC, Canada

THIRD INTERNATIONAL SYMPOSIUM
ON C-H ACTIVATION

May 30 – June 2, 2016

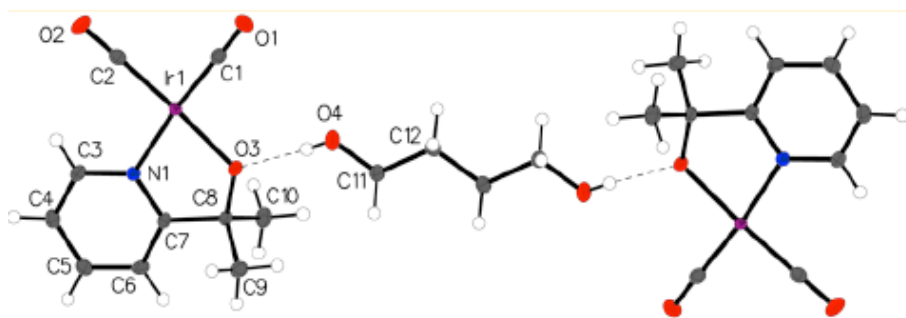
IL18 – 'Blue Solution': Hydrocarbon Oxidation and Structural Study

Daria Huang,^a Stafford Sheehan,^a David Balcells,^{*b} Gary W. Brudvig,^{*a} Victor S. Batista,^{*a}
and Robert H. Crabtree^{*a}

Department of Chemistry, Yale University, 225 Prospect St., New Haven, CT, 06520, USA
Univ Oslo, Dept Chem, CTCC, N-0315 Oslo, Norway

E-mail: robert.crabtree@yale.edu

A variety of organometallic Ir(I) and (III) precursors undergo oxidation to give Ir(IV) oxo complexes that act as resting states for oxidation catalysis, either hydrocarbon oxidation or water oxidation. Hydrocarbon oxidation proceeds with retention of configuration at carbon, consistent with a concerted oxene type insertion. For one such precursor, the Ir(I) dicarbonyl shown below, structural study required a diol crystallization agent which hydrogen bonds to the alkoxide lone pair.



References

1. Huang, D.; Beltrán-Suito, R.; Thomsen, J.; Hashmi, S.; Materna, K.; Sheehan, S.; Mercado, B.; Brudvig, G. W.; Crabtree, R. H. *Inorg. Chem.* **2016**, *55*, 2427-2435.
2. Sinha, S. B.; Shopov, D.; Sharninghausen, L.; Vinyard, D.; Mercado, B.; Brudvig, G. W.; Crabtree, R. H. *J. Am. Chem. Soc.* **2015**, *138*, 15692-15695.
3. Shopov, D.; Rudshiteyn, B.; Campos, J.; Batista, V. S.; Crabtree, R. H.; Brudvig, G. W. *J. Am. Chem. Soc.* **2015**, *137*, 7243-7250.
4. Crabtree, R.H., A. *J. Organometal. Chem.* **2015**, *793*, 41-46.
5. Sheehan, S. W.; Thomsen, J. M.; Hintermair, U.; Crabtree, R. H.; Brudvig, G. W.; Schmittenmaer, C. A. *Nature Commun.* **2015**, *5*, 6469.