

SUPPLEMENTARY MATERIAL

A mechanistic study of acetate-assisted C-H activation of 2-substituted pyridines with $[MCl_2Cp^*]_2$ ($M = Rh, Ir$) and $[RuCl_2(p\text{-cymene})]_2$.

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Table 1. Crystal data for $[RuCl\{C_5H_4N\text{-}2\text{-}C(=O)CH_3\text{-}K\text{N},O\}(p\text{-cymene})]PF_6$. (4c)

| | | | |
|-----------------------------------|--|--------------------------|--|
| Empirical formula | C17.50 H22 Cl2 F6 N O P Ru | | |
| Formula weight | 579.30 | | |
| Temperature | 150(2) K | | |
| Crystal system | Triclinic | | |
| Space group | P-1 | | |
| Unit cell dimensions | $a = 8.2642(13)$ Å | $\alpha = 108.431(3)$ °. | |
| | $b = 11.6003(18)$ Å | $\beta = 101.315(3)$ °. | |
| | $c = 12.534(2)$ Å | $\gamma = 102.736(3)$ °. | |
| Volume | $1065.0(3)$ Å ³ | | |
| Z | 2 | | |
| Density (calculated) | 1.806 Mg/m ³ | | |
| Absorption coefficient | 1.123 mm ⁻¹ | | |
| F(000) | 578 | | |
| Crystal size | 0.16 x 0.14 x 0.07 mm ³ | | |
| Theta range for data collection | 1.79 to 26.00°. | | |
| Index ranges | $-10 \leq h \leq 10, -14 \leq k \leq 14, -15 \leq l \leq 14$ | | |
| Reflections collected | 8430 | | |
| Independent reflections | 4161 [R(int) = 0.0318] | | |
| Completeness to theta = 26.00° | 99.1 % | | |
| Absorption correction | Empirical | | |
| Max. and min. transmission | 0.956 and 0.816 | | |
| Refinement method | Full-matrix least-squares on F ² | | |
| Data / restraints / parameters | 4161 / 0 / 257 | | |
| Goodness-of-fit on F ² | 0.978 | | |
| Final R indices [I>2sigma(I)] | R1 = 0.0393, wR2 = 0.0800 | | |
| R indices (all data) | R1 = 0.0488, wR2 = 0.0827 | | |
| Largest diff. peak and hole | 1.008 and -0.507 e.Å ⁻³ | | |