Palladium-catalyzed Direct and Regioselective C-H Acyloxylation of Indolizines

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**B3LYP/6-31+G(d,p) Optimized Geometries and Atomic charges in 3-methoxycarbonylindolizine**

Method: DFT, functional B3LYP, basis set 6-311+G(d,p), gas phase

Mulliken atomic charges at carbon atoms:

Mulliken charges with hydrogens summed into their linked carbon atoms:

**B3LYP/6-31+G(d,p) Optimized Geometries and Atomic charges in Methyl indolizine-2-carboxylate**

Method: DFT, functional B3LYP, basis set 6-311+G(d,p), gas phase

Mulliken atomic charges at carbon atoms:

Mulliken charges with hydrogens summed into their linked carbon atoms:
ORTEP drawing of $2t$ (CCDC 1049376)