Supporting Information for

"Spectroscopy and Electronic Structures of $Ru_2(ap)_4$-alkynyl Compounds"

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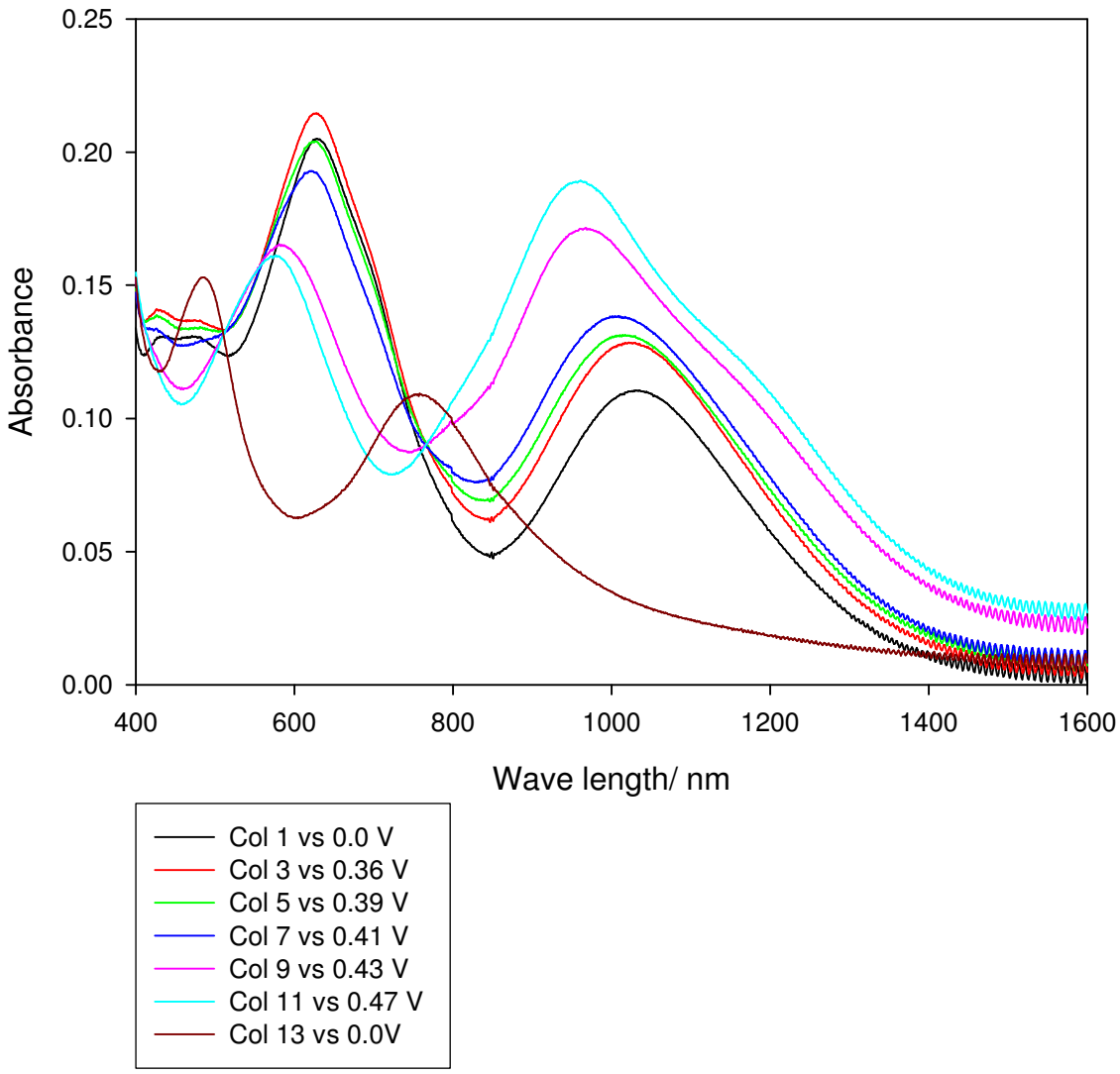
Preparation of 2-(3-^{i}butoxyanilino)pyridine (H^{t}BuOap).

(a) *(3-^{i}butoxy-phenyl)-carbamic acid tert-butyl ester.* A mixture of 3-(*N*-*t*-butyloxycarbonylamino)phenol (8.2 g, 39 mmol), 1-bromo-2-methylpropoane (7.0 mL, 64 mmol), potassium carbonate (15.0 g, 108 mmol) and NaI (0.50 g, 3.3 mmol) in 250 mL dimethylformamide was stirred at 60 ˚C for 48 h. The reaction mixture was poured into ice water, and extracted with ethyl acetate. The organic phase was washed with brine and dried over Na_2SO_4. Brown oil was obtained upon the solvent removal. Recrystallization in CH_2Cl_2 and hexanes afforded (3-^{i}butoxy-phenyl)-carbamic acid tert-butyl ester as white crystals (9.6 g, 92%). ^{1}H NMR: 7.18-7.10 (m, 1H, aromatic), 6.80-6.47 (m, 3H, aromatic), 3.72-3.69 (m, 2H, $OC\underline{H_2}CH(CH_3)_2$), 2.05 (s, 1H, $OCH_2C\underline{H}(CH_3)_2$), 1.55-1.52 (m, 9H, $OC(C\underline{H_3})_3$), 1.03-1.00 (m, 6H, $OCH_2CH(C\underline{H_3})_2$).

(b) 3-Isobutoxy-aniline. To a solution of (3-isobutoxy-phenyl)-carbamic acid tert-butyl ester (1.49 g, 5.6 mmol) in 30 mL dichloromethane, trifluoroacetic acid(1 mL, 13.5 mmol) was added at 0 ˚C. Then the solution was warmed to room temperature, and was

stirred overnight. After neutralization with NaOH solution, the reaction mixture was extracted with CH_2Cl_2. The organic layer was washed with brine and dried over Na_2SO_4. Upon solvent removal, brown oil was obtained (0.89 g, 57%). ^{1}H NMR: 7.24-7.17 (m, 1H, aromatic), 6.77-6.72 (m, 3H, aromatic), 3.65 (d, *J*=3.2Hz, 2H, $OC\underline{H_2}CH(CH_3)_2$), 2.07-1.98 (m, 1H, $OCH_2C\underline{H}(CH_3)_2$), 1.00-0.97 (m, 6H, $OCH_2CH(C\underline{H_3})_2$).



The figure shows that when you oxidized **3**, you get the spectrum of oxidized **2** (Figure 7a). Upon reduction (col 13 vs 0.0 V), one gets the spectrum of **2** (Figure 8)