Supporting Information

Ruthenium-catalyzed estragole isomerization: high *trans*-selective formation of anethole.

Beatriz Lastra-Barreira, Pascale Crochet*

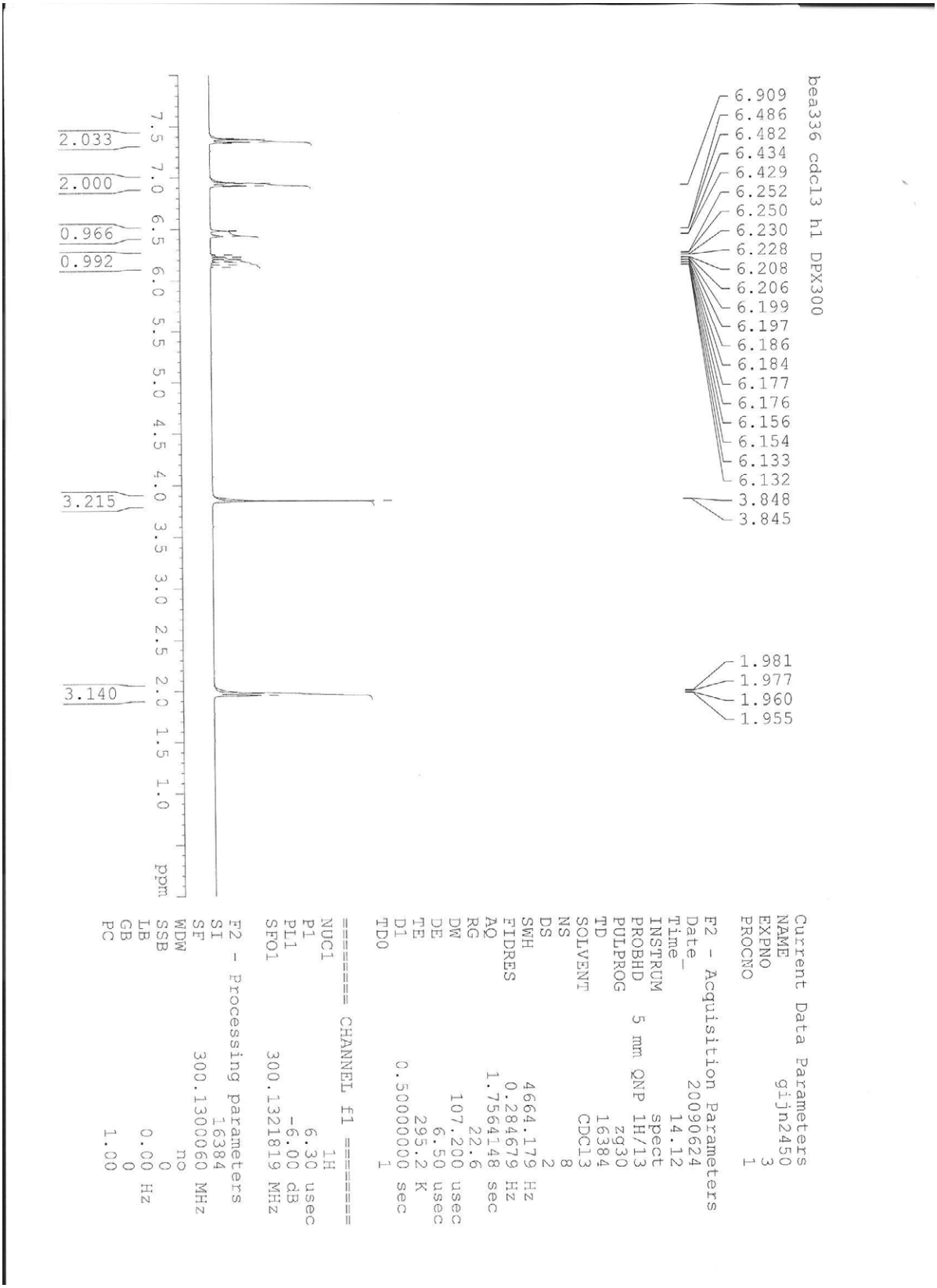
Departamento de Química Orgánica e Inorgánica, Instituto Universitario de Química Organometálica "Enrique Moles" (Unidad Asociada al CSIC), Facultad de Química, Universidad de Oviedo, E-33071 Oviedo, Spain. Fax: (+34)-985 10 34 46, e-mail: crochetpascale@uniovi.es.

Spectroscopic data of *trans*-anethole. ^{1}H NMR, $CDCl_3$, δ: 7.32 and 6.89 (both d, 2 H each, $^{3}J_{HH}$ = 8.8 Hz, $CH_{aromatics}$), 6.41 (broad d, 1 H, $^{3}J_{HH}$ = 15.7 Hz, CH=), 6.15 (dq, 1 H, $^{3}J_{HH}$ = 15.7 Hz, $^{3}J_{HH}$ = 6.6 Hz, =C*H*Me), 3.84 (s, 3 H, OMe), 1.92 (dd, 3 H, $^{3}J_{HH}$ = 6.6 Hz, $^{4}J_{HH}$ = 1.4 Hz, =CH*Me*). $^{13}C\{^{1}H\}$ NMR, $CDCl_3$, δ: 159.1 and 131.8 ($C_{aromatics}$), 131.0 and 123.8 (CH=), 127.4 and 114.4 ($C_{aromatics}$), 55.6 (OMe), 18.9 (Me).

Spectroscopic data of *cis*-anethole: ^{1}H NMR, $CDCl_3$, δ: 5.77 (dq, 1 H, $^{3}J_{HH}$ = 11.5 Hz, $^{3}J_{HH}$ = 7.1 Hz, =C*H*Me), 3.85 (s, 3 H, OMe), 1.96 (dd, 3 H, $^{3}J_{HH}$ = 7.1 Hz, $^{4}J_{HH}$ = 1.8 Hz, =CH*Me*). The other signals are partially overlapped by those of *trans*-anethole, always presents as the major product.

Chromatographic analyses: GC analyses have been performed on an Hewlett-Packard HP6890 apparatus equipped with a flame ionization detector (FID) and a capillary Supelco Beta-Dex^{TM} 120 column (30 m length, 250 μm diameter), using a 4 mL/min flow of helium. *Temperature program used*: initial temperature, 160ºC; heating, 10ºC/min; final temperature, 210ºC. *Retention times*: t_R(estragole) = 1.76 min; t_R(*trans*-anethole) = 2.01 min; t_R(*cis*-anethole) = 2.19 min.

^{1}H NMR spectrum of isolated *trans*-anethole (in $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR spectrum of isolated *trans*-anethole (in $CDCl_3$)