

Supporting Information

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

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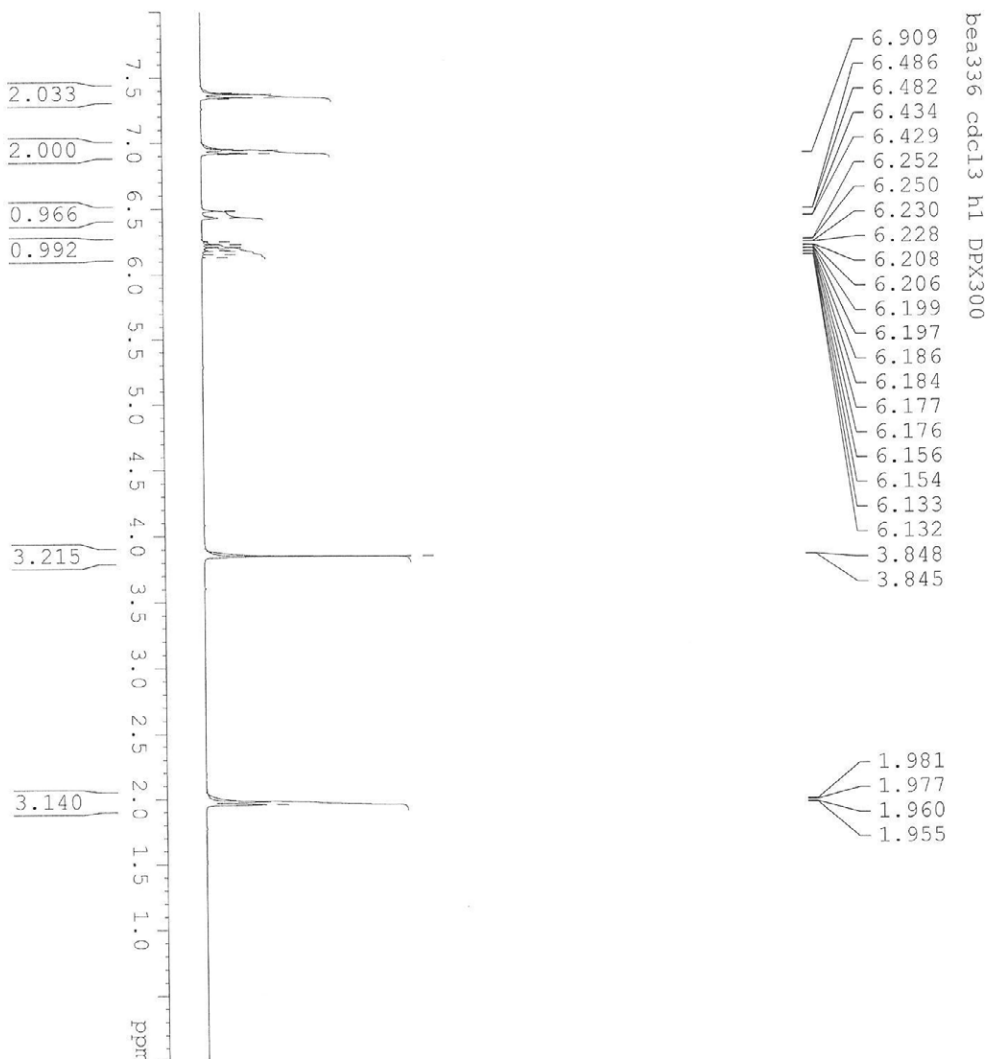
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Spectroscopic data of *trans*-anethole. ^1H NMR, CDCl_3 , δ : 7.32 and 6.89 (both d, 2 H each, $^3J_{\text{HH}} = 8.8$ Hz, $\text{CH}_{\text{aromatics}}$), 6.41 (broad d, 1 H, $^3J_{\text{HH}} = 15.7$ Hz, $\text{CH}=\text{}$), 6.15 (dq, 1 H, $^3J_{\text{HH}}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

Spectroscopic data of *cis*-anethole: ^1H NMR, CDCl_3 , δ : 5.77 (dq, 1 H, $^3J_{\text{HH}} = 11.5$ Hz, $^3J_{\text{HH}} = 7.1$ Hz, $=\text{CHMe}$), 3.85 (s, 3 H, OMe), 1.96 (dd, 3 H, $^3J_{\text{HH}} = 7.1$ Hz, $^4J_{\text{HH}} = 1.8$ Hz, $=\text{CHMe}$). 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-DexTM 120 column (30 m length, 250 μm diameter), using a 4 mL/min flow of helium. *Temperature program used:* initial temperature, 160°C; heating, 10°C/min; final temperature, 210°C. *Retention times:* $t_{\text{R}}(\text{estragole}) = 1.76$ min; $t_{\text{R}}(\text{trans-anethole}) = 2.01$ min; $t_{\text{R}}(\text{cis-anethole}) = 2.19$ min.

¹H NMR spectrum of isolated *trans*-anethole (in CDCl₃)



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 PROCNO 1

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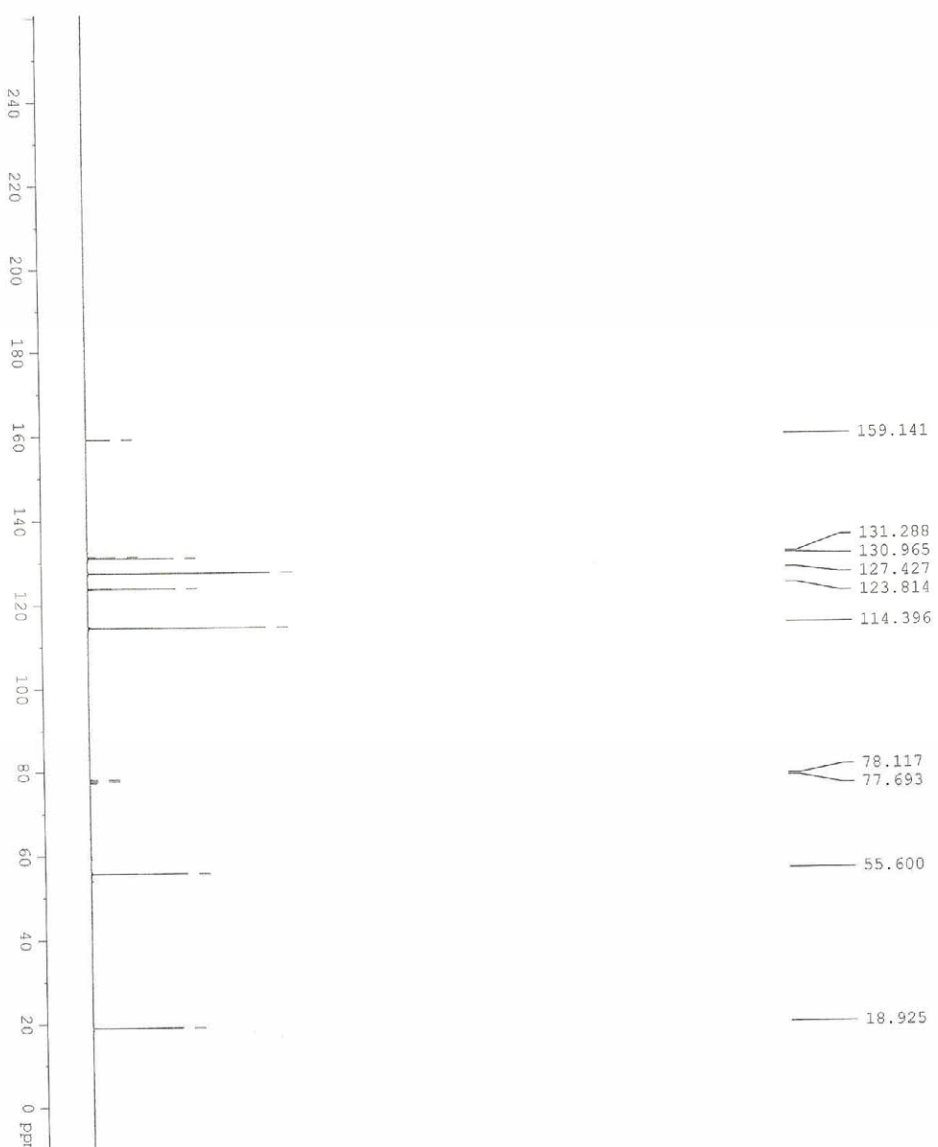
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F2 - Processing parameters

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 PC 1.00

¹³C{¹H} NMR spectrum of isolated *trans*-anethole (in CDCl₃)



bea336 cdcl3 C13 CPD DPX300

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 d11 0.03000000 sec
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 PL12 21.00 dB
 PL13 120.00 dB
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F2 - Processing parameters
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