

Electronic supporting information

Reactivity of Diatomics and of Ethylene on Zeolite-Supported 13-Atom Platinum Nanoclusters

Melanie Keppeler,^{†,1} Gabriele Bräuning,[†] Shankara Gayathri Radhakrishnan,[‡] Xiong Liu,^{†2} Christopher Jensen^{†3} and Emil Roduner^{†‡*}

[†] Institut für Physikalische Chemie, Universität Stuttgart,
Pfaffenwaldring 55, D-70569 Stuttgart, Germany

[‡] Department of Chemistry, University of Pretoria, Pretoria 0002, Republic of South Africa

*Corresponding author: e.roduner@ipc.uni-stuttgart.de

¹ Present address: Eichenweg 5c, D-89290 Buch, Germany

² Present address: Faculty of Materials Science and Engineering, Hubei University,
No. 368 Youyi Avenue, Wuchang, Wuhan 430062, China

³ Present address: ThyssenKrupp Industrial Solutions AG, Business Unit Process Technologies,
Neubeckumer Straße 127, D-59320 Ennigerloh, Germany

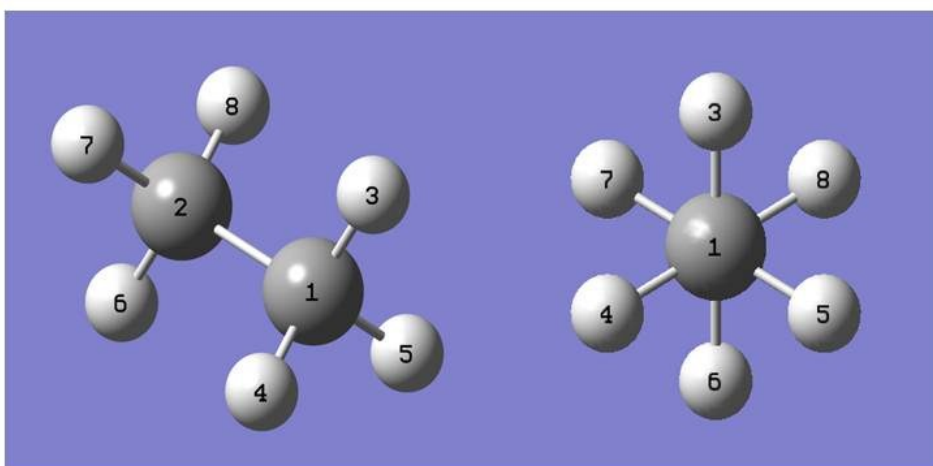


Figure S1: Numbering Scheme of ethane molecule. All isotopomers were calculated for staggered conformations (back rotor rotated by 60° with respect to front rotor). Eclipsed conformations exhibited negative frequencies for the lowest frequency (internal rotation) mode.

Table S1: Calculated intensities for various isotopologues in different conformations for the ethane product

| Isotopologue | Conformation | Vibrational frequency / cm ⁻¹ | Intensity |
|---|--------------|---|-----------|
| CH ₃ -CH ₃ | staggered | 307.22 | 0.0000 |
| | | 826.26 | 3.6934 |
| | | 826.26 | 3.9634 |
| | | 994.71 | 0.0000 |
| | | 1220.84 | 0.0000 |
| | | 1220.85 | 0.0000 |
| | | 1412.54 | 0.9735 |
| | | 1422.11 | 0.0000 |
| | | 1502.94 | 0.0000 |
| | | 1502.94 | 0.0000 |
| | | 1505.73 | 9.1539 |
| | | 1505.73 | 9.1539 |
| | | 3025.71 | 0.0000 |
| | | 3026.16 | 59.5319 |
| | | 3071.27 | 0.0000 |
| | | 3071.27 | 0.0000 |
| 3096.26 | 62.8088 | | |
| 3096.26 | 62.7977 | | |
| CH ₂ D-CH ₃ Atom 5 = D | staggered | 288.30 | 0.0013 |
| | | 718.67 | 2.2116 |
| | | 810.58 | 3.9376 |
| | | 979.98 | 0.2446 |
| | | 1138.52 | 0.7438 |
| | | 1183.73 | 0.1900 |
| | | 1326.64 | 1.3827 |
| | | 1335.09 | 2.4385 |
| | | 1417.49 | 0.4589 |
| | | 1481.43 | 3.0084 |
| | | 1504.22 | 6.0828 |
| | | 1504.29 | 4.4416 |
| | | 2246.51 | 14.9967 |
| | | 3025.93 | 29.3394 |
| 3045.25 | 23.5320 | | |
| 3071.07 | 0.0011 | | |

| | | | |
|--|---------------|---------|---------|
| | | 3085.36 | 38.9545 |
| | | 3096.12 | 62.5433 |
| CH ₂ D-CH ₂ D Atoms 5,7 = D | D-D staggered | 268.37 | 0.0013 |
| | | 637.45 | 1.9366 |
| | | 749.04 | 3.0521 |
| | | 972.74 | 0.3755 |
| | | 1062.60 | 1.0520 |
| | | 1137.59 | 0.7477 |
| | | 1301.71 | 1.3737 |
| | | 1309.68 | 0.3576 |
| | | 1338.71 | 3.4294 |
| | | 1350.42 | 2.5363 |
| | | 1478.97 | 2.2963 |
| | | 1484.59 | 6.4313 |
| | | 2243.39 | 16.3973 |
| | | 2249.58 | 13.6002 |
| | | 3043.63 | 38.9012 |
| | | 3047.47 | 10.3005 |
| | | 3078.71 | 22.9714 |
| | | 3094.72 | 51.4465 |
| CH ₂ D-CH ₂ D Atoms 5,7 = D | D-D anti | 267.38 | 0.0046 |
| | | 662.01 | 1.8646 |
| | | 796.87 | 4.1357 |
| | | 909.90 | 0.0000 |
| | | 1071.14 | 0.0000 |
| | | 1153.04 | 0.0000 |
| | | 1302.20 | 3.4952 |
| | | 1310.88 | 5.0261 |
| | | 1339.11 | 0.0000 |
| | | 1351.06 | 0.0000 |
| | | 1478.41 | 0.0000 |
| | | 1485.14 | 9.0212 |
| | | 2242.73 | 0.0000 |
| | | 2250.19 | 30.7581 |
| | | 3042.00 | 0.0000 |
| | | 3051.58 | 60.6113 |
| | | 3070.88 | 0.0000 |
| | | 3095.98 | 62.2889 |
| CHD ₂ -CH ₃ Atoms 4,5 = D | staggered | 275.43 | 0.0007 |
| | | 687.91 | 2.0985 |

| | | | |
|---|---------------|---------|---------|
| | | 741.58 | 2.9254 |
| | | 948.63 | 0.6783 |
| | | 1100.86 | 1.3484 |
| | | 1132.35 | 0.8107 |
| | | 1142.74 | 0.3593 |
| | | 1329.97 | 4.3955 |
| | | 1331.01 | 0.8364 |
| | | 1417.51 | 0.4335 |
| | | 1503.32 | 4.9948 |
| | | 1503.94 | 4.5055 |
| | | 2209.71 | 14.9540 |
| | | 2284.76 | 14.9397 |
| | | 3025.93 | 29.6458 |
| | | 3060.79 | 11.1281 |
| | | 3083.91 | 32.0227 |
| | | 3088.60 | 51.1283 |
| CH ₂ D-CHD ₂ Atoms 5,6,8 = D | H-D staggered | 253.87 | 0.0026 |
| | | 637.52 | 1.7756 |
| | | 725.65 | 3.0357 |
| | | 903.51 | 0.1650 |
| | | 1032.51 | 0.7958 |
| | | 1094.97 | 0.6166 |
| | | 1122.14 | 1.2213 |
| | | 1296.96 | 1.7922 |
| | | 1321.15 | 3.1804 |
| | | 1331.50 | 3.1626 |
| | | 1350.76 | 1.4002 |
| | | 1481.68 | 4.6317 |
| | | 2209.69 | 14.8563 |
| | | 2245.77 | 12.8782 |
| | | 2285.40 | 17.9560 |
| | | 3046.17 | 22.3305 |
| | | 3062.37 | 22.1663 |
| | | 3087.36 | 47.9358 |
| CH ₂ D-CHD ₂ Atoms 5,6,8 = D | H-D anti | 254.55 | 0.0001 |
| | | 660.77 | 2.0580 |
| | | 678.75 | 2.2427 |
| | | 947.96 | 0.6605 |
| | | 1028.78 | 0.3809 |
| | | 1099.15 | 1.2643 |

| | | | |
|---|-----------|---------|---------|
| | | 1102.16 | 1.4740 |
| | | 1305.97 | 0.2502 |
| | | 1315.94 | 0.0082 |
| | | 1337.11 | 6.9191 |
| | | 1339.68 | 2.2151 |
| | | 1481.69 | 4.3513 |
| | | 2209.19 | 15.3365 |
| | | 2246.95 | 14.5722 |
| | | 2284.85 | 14.9863 |
| | | 3044.85 | 28.9238 |
| | | 3067.58 | 32.5204 |
| | | 3083.58 | 31.7395 |
| CH ₃ -CD ₃ Atoms 3,4,5 = D | staggered | 266.29 | 0.0000 |
| | | 681.86 | 2.2972 |
| | | 681.86 | 2.2980 |
| | | 907.31 | 0.0346 |
| | | 1082.87 | 2.8191 |
| | | 1082.87 | 2.8204 |
| | | 1132.95 | 0.4701 |
| | | 1132.95 | 0.4702 |
| | | 1135.16 | 0.4019 |
| | | 1417.41 | 0.4455 |
| | | 1503.08 | 4.6843 |
| | | 1503.09 | 4.6867 |
| | | 2174.08 | 14.9609 |
| | | 2284.72 | 14.8528 |
| | | 2284.72 | 14.8495 |
| | | 3025.93 | 29.7367 |
| | | 3083.91 | 32.0404 |
| | | 3083.91 | 32.0348 |
| CD ₃ -CD ₃ | staggered | 217.32 | 0.0000 |
| | | 597.15 | 1.8775 |
| | | 597.15 | 1.8781 |
| | | 845.32 | 0.0000 |
| | | 979.97 | 0.0000 |
| | | 979.97 | 0.0000 |
| | | 1074.77 | 0.0000 |
| | | 1074.77 | 0.0000 |
| | | 1079.52 | 0.7536 |
| | | 1091.55 | 5.7504 |

| | | | |
|--|--|---------|---------|
| | | 1091.56 | 5.7531 |
| | | 1163.92 | 0.0000 |
| | | 2171.32 | 29.9004 |
| | | 2176.80 | 0.0000 |
| | | 2276.90 | 0.0000 |
| | | 2276.90 | 0.0000 |
| | | 2292.41 | 31.0437 |
| | | 2292.41 | 31.0370 |