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**Electronic supplementary material**

**Application of spectral graph theory on the enthalpy of formation of acyclic saturated ketones**

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Example of calculation of Δ*H*f.





*n*=7 *M*2=12 *M*4=40 *M*6=144 *M*8=544 *M*10=2112 *M*12=8320





*n*=7 *M*2=18 *M*4=94 *M*6=540 *M*8=3262 *M*10=20178 *M*12=126148





*n*=7 *M*2=13.08 *M*4=47.03 *M*6=181.77 *M*8=736.25 *M*10=3066.00 *M*12=12996.86



Calculated spectral moments up to *M*12 for case a) for molecules from Table I.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *M*0 | *M*2 | *M*4 | *M*6 | *M*8 | *M*10 | *M*12 |
| 4 | 6 | 18 | 54 | 162 | 486 | 1458 |
| 5 | 8 | 24 | 80 | 272 | 928 | 3168 |
| 6 | 10 | 30 | 100 | 350 | 1250 | 4500 |
| 6 | 10 | 30 | 106 | 390 | 1450 | 5406 |
| 7 | 12 | 36 | 120 | 420 | 1512 | 5532 |
| 7 | 12 | 36 | 126 | 468 | 1782 | 6858 |
| 8 | 14 | 42 | 146 | 546 | 2114 | 8322 |
| 10 | 18 | 54 | 180 | 630 | 2268 | 8316 |
| 10 | 18 | 54 | 186 | 686 | 2638 | 10410 |
| 12 | 21 | 61 | 207 | 757 | 2891 | 11347 |
| 13 | 24 | 72 | 240 | 840 | 3024 | 11088 |
| 6 | 10 | 34 | 130 | 514 | 2050 | 8194 |
| 7 | 12 | 48 | 216 | 1008 | 4752 | 22464 |
| 7 | 12 | 40 | 156 | 640 | 2672 | 11224 |
| 7 | 12 | 40 | 144 | 544 | 2112 | 8320 |
| 7 | 12 | 40 | 156 | 640 | 2672 | 11224 |
| 8 | 14 | 54 | 248 | 1198 | 5874 | 28932 |
| 8 | 14 | 54 | 224 | 974 | 4354 | 19764 |
| 8 | 14 | 54 | 242 | 1142 | 5494 | 26622 |
| 8 | 14 | 50 | 206 | 898 | 4014 | 18146 |
| 9 | 16 | 64 | 304 | 1536 | 7936 | 41344 |
| 9 | 16 | 64 | 292 | 1408 | 6976 | 35032 |
| 10 | 18 | 78 | 396 | 2142 | 11898 | 66852 |
| 10 | 18 | 78 | 378 | 1926 | 10098 | 53838 |
| 10 | 18 | 62 | 234 | 934 | 3858 | 16286 |
| 11 | 20 | 84 | 386 | 1844 | 9010 | 44730 |
| 12 | 22 | 90 | 394 | 1794 | 8362 | 39570 |

Calculated spectral moments up to M12 for case b) for molecules from Table I.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *M*0 | *M*2 | *M*4 | *M*6 | *M*8 | *M*10 | *M*12 |
| 4 | 8 | 32 | 12 | 512 | 2048 | 9132 |
| 5 | 14 | 78 | 476 | 2942 | 18214 | 112788 |
| 6 | 16 | 84 | 496 | 3044 | 18896 | 117684 |
| 6 | 16 | 84 | 520 | 3300 | 21016 | 133908 |
| 7 | 18 | 90 | 516 | 3114 | 19188 | 119220 |
| 7 | 18 | 90 | 540 | 3402 | 21708 | 138996 |
| 8 | 20 | 96 | 560 | 3504 | 22400 | 144096 |
| 10 | 24 | 108 | 576 | 3324 | 19944 | 122040 |
| 10  | 24 | 108 | 600 | 3644 | 22984 | 147192 |
| 12 | 27 | 115 | 621 | 3715 | 23237 | 148165 |
| 13 | 30 | 126 | 636 | 3534 | 20700 | 124812 |
| 6 | 16 | 88 | 544 | 3472 | 22336 | 143968 |
| 7 | 18 | 102 | 648 | 4302 | 28998 | 196452 |
| 7 | 18 | 94 | 570 | 3622 | 23378 | 151678 |
| 7 | 18 | 94 | 540 | 3262 | 20178 | 126148 |
| 7 | 18 | 94 | 588 | 3838 | 25298 | 167140 |
| 8  | 20 | 108 | 680 | 4516 | 30600 | 208932 |
| 8 | 20 | 108 | 620 | 3716 | 22900 | 143532 |
| 8 | 20 | 108 | 692 | 4676 | 32140 | 222156 |
| 8 | 20 | 104 | 656 | 4384 | 29760 | 202880 |
| 9 | 22 | 118 | 736 | 4878 | 33202 | 228724 |
| 9 | 22 | 118 | 760 | 5230 | 36802 | 260932 |
| 10 | 24 | 132 | 828 | 5508 | 37764 | 263196 |
| 10 | 24 | 132 | 864 | 6084 | 44064 | 322596 |
| 10 | 24 | 116 | 684 | 3940 | 24984 | 161492 |
| 11 | 26 | 138 | 836 | 5450 | 36916 | 255060 |
| 12 | 28 | 144 | 808 | 4848 | 30448 | 196800 |

Calculated spectral moments up to M12 for case c) for molecules from Table I.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| *M*0 | *M*2 | *M*4 | *M*6 | *M*8 | *M*10 | *M*12 |
| 4 | 7.08 | 25.03 | 88.54 | 313.23 | 1109.09 | 39193.97 |
| 5 | 9.08 | 31.03 | 117.77 | 455.65 | 1768.70 | 6869.41 |
| 6 | 11.08 | 37.03 | 137.77 | 537.95 | 2141.98 | 8593.25 |
| 6 | 11.08 | 37.03 | 146.99 | 606.07 | 2520.07 | 10499.17 |
| 7 | 13.08 | 43.03 | 157.77 | 607.95 | 2409.35 | 9699.68 |
| 7 | 13.08 | 43.03 | 166.99 | 688.37 | 2903.34 | 12355.92 |
| 8 | 15.08 | 49.03 | 186.99 | 770.67 | 3286.62 | 14224.67 |
| 10 | 19.08 | 61.03 | 217.77 | 817.95 | 3165.35 | 12490.14 |
| 10 | 19.08 | 61.03 | 226.99 | 910.67 | 3821.37 | 16461.54 |
| 12 | 22.08 | 68.03 | 247.99 | 981.67 | 4074.37 | 17404.99 |
| 13 | 25.08 | 79.03 | 277.77 | 1027.95 | 3921.35 | 15262.14 |
| 6 | 11.08 | 41.03 | 170.99 | 738.67 | 3222.62 | 14096.67 |
| 7 | 13.08 | 55.03 | 260.22 | 12823.29 | 6402.09 | 32092.48 |
| 7 | 13.08 | 47.03 | 196.99 | 868.97 | 3906.64 | 17686.74 |
| 7 | 13.08 | 47.03 | 181.77 | 736.25 | 3066.00 | 12966.86 |
| 7 | 13.08 | 47.03 | 200.22 | 897.09 | 4084.74 | 18696.58 |
| 8 | 15.08 | 61.03 | 292.22 | 1476.59 | 7596.87 | 3932.47 |
| 8 | 15.08 | 61.03 | 261.77 | 1170.55 | 5380.78 | 25164.95 |
| 8 | 15.08 | 61.03 | 289.45 | 1448.71 | 7394.96 | 38024.33 |
| 8 | 15.08 | 57.03 | 253.45 | 1196.11 | 5780.15 | 28201.92 |
| 9 | 17.08 | 71.03 | 348.22 | 1818.89 | 9742.40 | 52719.84 |
| 9 | 17.08 | 71.03 | 342.67 | 1755.73 | 9241.13 | 49247.42 |
| 10 | 19.08 | 85.03 | 440.22 | 2429.19 | 13798.68 | 79460.27 |
| 10 | 19.08 | 85.03 | 431.90 | 2323.35 | 12872.86 | 72468.46 |
| 10 | 19.08 | 69.03 | 274.99 | 1167.27 | 5154.67 | 23321.71 |
| 11 | 21.08 | 91.03 | 433.45 | 2163.61 | 11097.04 | 57948.00 |
| 12 | 23.08 | 97.03 | 434.99 | 2035.87 | 9804.23 | 48139.68 |



Fig. S1. Dependence of the enthalpy of formation on the branching of molecule in 2-nonanones.



Fig. S2. Dependence of the enthalpy of formation on the branching of molecule in 4-nonanones.

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