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SUPPLEMENTARY MATERIAL TO

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

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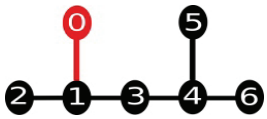
EXAMPLES OF THE CALCULATION OF ΔH_f



$$\begin{bmatrix} 0&1&0&0&0&0&0\\ 1&0&1&1&0&0&0\\ 0&1&0&0&0&0&0\\ 0&1&0&0&1&0&0\\ 0&0&0&1&0&1&1\\ 0&0&0&0&1&0&0\\ 0&0&0&0&1&0&0 \end{bmatrix}$$

n=7 M_2=12 M_4=40 M_6=144 M_8=544 M_{10}=2112 M_{12}=8320M$_6$

$$\Delta H_f \approx -39.29136 \cdot 7 + 17.68924 \cdot 12 - 2.65522 \cdot 40 - 1.74032 \cdot 144\ 1.08415 \cdot 544 -$$
$$- 0.23210 \cdot 2112 + 0.01749 \cdot 8320 - 117.23579 \ - 291.72 \text{ kJ mol}^{-1}$$

$$\begin{bmatrix} 0&2&0&0&0&0&0\\ 2&0&1&1&0&0&0\\ 0&1&0&0&0&0&0\\ 0&1&0&0&1&0&0\\ 0&0&0&1&0&1&1\\ 0&0&0&0&1&0&0\\ 0&0&0&0&1&0&0 \end{bmatrix}$$

n=7 M_2=18 M_4=94 M_6=540 M_8=3262 M_{10}=20178 M_{12}=126148

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$$\Delta H_f \approx -39.29136 \cdot 7 + 17.68924 \cdot 18 - 2.65522 \cdot 94 - 1.74032 \cdot 540 + 1.08415 \cdot 3262 -$$
$$- 0.23210 \cdot 20178 + 0.01749 \cdot 126148 - 117.23579 = -203.72 \text{ kJ mol}^{-1}$$

$$\begin{bmatrix} 0 & 1.24 & 0 & 0 & 0 & 0 & 0 \\ 1.24 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

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

$$\Delta H_f \approx -39.29136 \cdot 7 + 17.68924 \cdot 13.08 - 2.65522 \cdot 47.03 - 1.74032 \cdot 181.77 +$$
$$+1.08415 \cdot 736.25 - 0.23210 \cdot 3066.00 + 0.01749 \cdot 12996.56 - 117.23579 =$$
$$= -288.74 \text{ kJ mol}^{-1}$$

TABLE S-I. 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

TABLE S-II. Calculated spectral moments up to M_{12} 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

TABLE S-III. Calculated spectral moments up to M_{12} 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

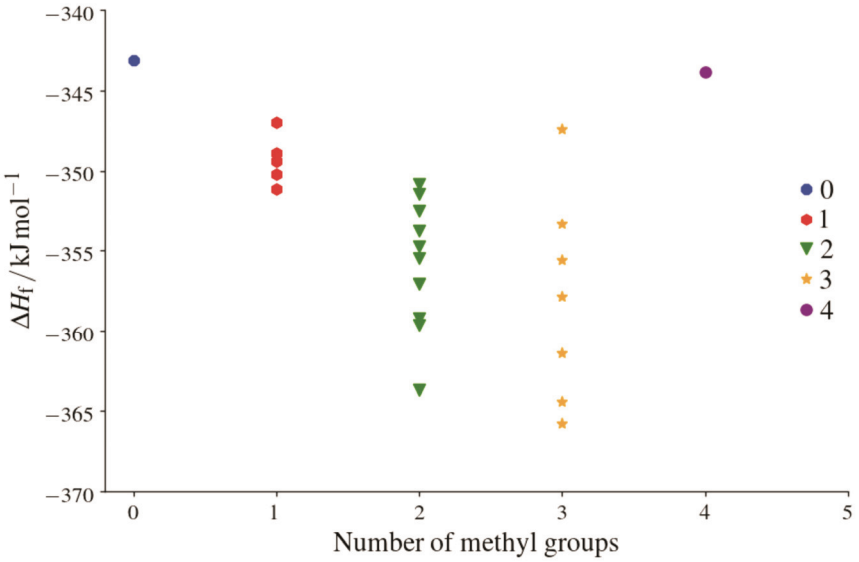

Fig. S-1. Dependence of the enthalpy of formation on the branching of the molecule in 2-nonanones.

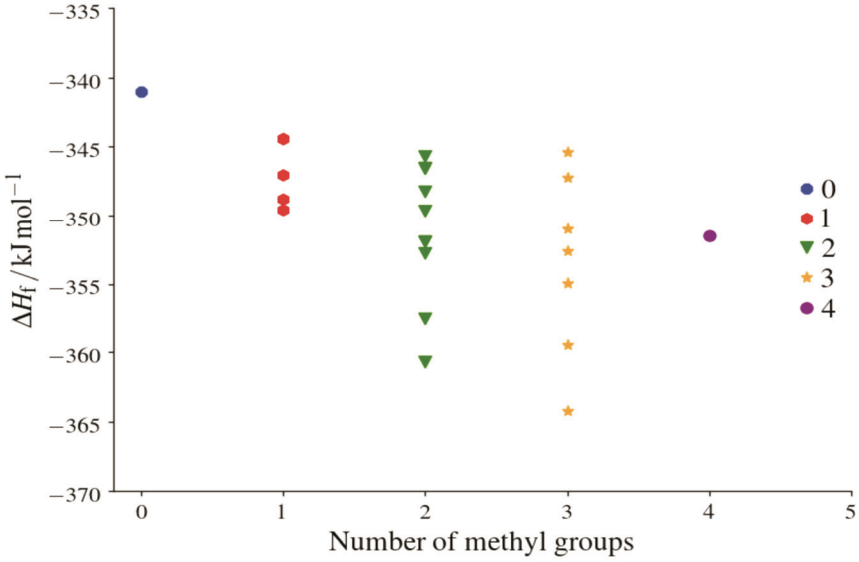

Fig. S-2. Dependence of the enthalpy of formation on the branching of the molecule in 4-nonanones.