INTERNATIONAL JOURNAL OF PHARMACEUTICAL, CHEMICAL AND BIOLOGICAL SCIENCES

Available online at www.ijpcbs.com

Research Article

DETERMINATION OF THERMODYNAMIC PROPERTIES OF SOME EUGENOL DERIVATIVES IN DIFFERENT SOLVENT MEDIA

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ABSTRACT

Thermodynamic properties (enthalpy (ΔH, kcal/mol), heat capacity (C, cal/Kmol), entropy (ΔS, cal/Kmol) and free energy (ΔG, kcal/mol)) of some eugenol derivatives (**(1)** 4-allyl-2-methoxy-6-(phenyldiazenyl)phenol, **(2)** 4-allyl-2-((4-hydroxyphenyl)diazenyl)-6-methoxy phenol, **(3)** 4-allyl-2-((4-iodophenyl)diazenyl)-6-methoxyphenol, **(4)** 4-((5-allyl-2-hydroxy-3-methoxy phenyl)diazenyl)benzenesulfonic acid) have been determined the MOPAC 2016 computer program at 298 K used in semi-empirical quantum chemical methods (PM7, PM6, PM6-DH2, RM1, PM3, AM1 and MNDO) in different solvents (methyl alcohol, ethyl alcohol, isopropyl alcohol, *n*-butyl alcohol, *tert*-butyl alcohol, ethylene glycol, dimetyl sulfoxide, ammonia, *N,N*-dimethyl formamide and acetonitrile). The results were evaluated by comparing between the solvents and the methods.

Keywords: Thermodynamic properties, semi-empirical quantum chemical methods.

INTRODUCTION

Eugenol is recognized by its characteristic flavor and aroma and by its medicinal, antimicrobial and antioxidant properties. But, the eugenol is unstable and sensitive to oxygen and is evaporable at low temperatures. So, their special properties not are effective in the preservations of the food when directly applied in the food or when applied as antimicrobial additive in food packaging.[1,2] Eugenol derivatives could be applied in many other areas if its thermal stability were improved. For example, eugenol can be used as an additive in the textile industry to manufacture antibacterial tissues for use in hospitals and laboratories and in the cellulose industry for the production of antibacterial papers. However, for these applications, the manufacturing processes involve temperatures that are higher than the volatilization temperature of eugenol.[3]

Thermodynamic first law is express clearly of the conservation of energy. Energy can thinkable a variety of forms such as thermal energy, chemical energy,kinetic energy or potential energy. The thermodynamic first law can be explainable for a closed system as

$$U = Q - W + ...$$

where U is the internal energy, Q is the thermal energy and W is the work performed by the system. Thermodynamic second law is states the entropy change

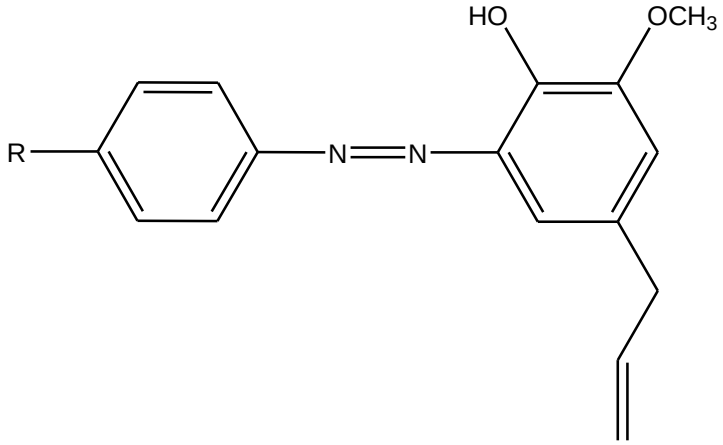
$$dS \geq \delta Q / T$$

where T is the absolute temperature of the system and δQ is the amount of heat transfered to the system.[4]

COMPUTATIONAL PART

MOPAC (Molecular Orbital Package) 2016 computer program is computational chemistry software with strong semi-empirical quantum chemistry practises for the prediction of chemical properties, calculations of chemical molecules and modelling of chemical reactions. MOPAC 2016 computer program is faster and highly reliable software for chemical property predictions and physical property predictions such as Gibbs free energies, activation energies, reaction paths, dipole moments, non-linear optical properties, enthalpy, heat capacity, entropy and infrared spectra. Also, MOPAC 2016 computer program implements the semi-empirical Hamiltonians PM7, PM6, PM6-DH2, RM1, PM3, AM1 and MNDO and combines the calculations of vibrational spectra, thermodynamic quantities, isotopic substitution effects, time-dependent effects, and force constants in a fully integrated program[5]. One of the usually used methods to search for the effect of substituent on an equilibrium proces is the

practice of the Hammett equation.[6] We calculated thermodynamic properties (enthalpy (ΔH, kcal/mol), heat capacity (C, cal/Kmol), entropy (ΔS, cal/Kmol) and free energy (ΔG, kcal/mol)) of this eugenol derivatives, molecule formüle for studied eugenol derivatives are given Fig. 1., with the MOPAC 2016 computer program at 298 K used in semi-empirical quantum chemical methods (PM7, PM6, PM6-DH2, RM1, PM3, AM1 and MNDO) in different solvents (methyl alcohol, ethyl alcohol, isopropyl alcohol, *n*-butyl alcohol, *tert*-butyl alcohol, ethylene glycol, dimetyl sulfoxide, ammonia, *N,N*-dimethyl formamide and acetonitrile). The data obtained as a result of calculations are given in Table 1. The graphical representation of the data obtained for molecule 1 is given in Figure 2.



Molecule	-R
1	-
2	-OH
3	-I
4	$-SHO_3$

Fig. 1: General molecule formüle for studied eugenol derivatives

Table 1: Calculated Enthalpy, Entropy, Heat Capacity and Free Energy values using semi-empirical quantum chemical methods with the MOPAC 2016 computer program at 298 K

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH, cal/mol)	Heat capacity (C, cal/Kmol)	Entropy (ΔS, cal/Kmol)	Free Energy (ΔG, kcal/mol)
Methanol (1)	PM7	12397.0308	72.3650	143.6457	-30430.9347
	PM6	12492.4486	74.2705	142.4146	-29968.4644
	PM6-DH2	12563.2090	74.0583	141.5078	-29627.3416
	RM1	12283.8998	71.9858	142.1116	-30086.6737
	PM3	12119.7724	71.4611	144.2051	-30874.9782
	AM1	12033.5584	69.9348	142.1866	-30359.3764
	MNDO	12178.0518	69.8993	143.4813	-30600.8978
Ethanol (1)	PM7	12417.9602	72.4296	145.0850	-30839.1326
	PM6	12717.6095	74.4498	148.2376	-31479.4309
	PM6-DH2	12530.3172	74.3208	143.5141	-30258.4117
	RM1	12183.6589	71.8519	140.5646	-29725.6766
	PM3	12139.4202	71.6154	143.5044	-30646.4167
	AM1	11981.9802	69.6538	141.7291	-30274.5510
	MNDO	12175.7410	69.8329	144.6039	-30937.9118
Iso-Propyl Alcohol (1)	PM7	12420.6270	72.5007	144.1616	-30561.1540
	PM6	12676.2246	74.4399	145.9678	-30844.0750
	PM6-DH2	12692.8805	74.4737	145.4023	-30658.8152
	RM1	12198.8978	71.9627	139.5945	-29421.2024
	PM3	12147.2978	71.6959	144.7526	-31010.6899
	AM1	12319.4426	70.1859	147.4833	-31652.7033
	MNDO	12264.5922	69.9139	146.8253	-31511.3710
n-butyl alcohol (1)	PM7	12425.5173	72.5010	144.7336	-30726.8060
	PM6	12577.8452	73.7346	147.8418	-31501.1870
	PM6-DH2	12523.3622	74.1107	144.8515	-30664.1130
	RM1	12176.1253	71.7557	141.8759	-30124.1740
	PM3	12198.5232	71.7265	144.3802	-30848.4330
	AM1	12059.7263	69.8605	144.5309	-31032.1620
	MNDO	12067.2085	69.6206	142.9549	-30554.7950

tert-butyl alcohol (1)	PM7	12565.0810	72.6973	146.2650	-31043.8288
	PM6	12653.3664	74.4344	145.3302	-30676.8327
	PM6-DH2	12536.5839	74.2230	143.7188	-30313.1763
	RM1	12202.5087	71.9204	139.9658	-29528.2946
	PM3	12172.6110	71.7478	142.6727	-30365.2545
	AM1	12241.0282	70.1593	146.8350	-31537.8271
	MNDO	12010.2452	69.3999	141.7590	-30255.2007
Solvent (Molecule)	**Method**	**Thermodynamic Properties**			
		Enthalpy (ΔH, kcal/mol)	**Heat capacity (C, cal/Kmol)**	**Entropy (ΔS, cal/Kmol)**	**Free Energy (ΔG, kcal/mol)**
Ethylene glycol (1)	PM7	12444.3372	72.4820	144.5059	-30640.0969
	PM6	12755.0713	74.6776	144.9584	-30464.2757
	PM6-DH2	12482.0590	74.1907	142.1669	-29905.0022
	RM1	11973.4921	70.9770	142.3979	-30482.4418
	PM3	12155.5411	71.5749	143.8843	-30743.5629
	AM1	12170.3014	70.0265	145.4780	-31203.9643
	MNDO	12168.1688	69.8622	143.1641	-30516.2076
Dimetyl sulfoxide (1)	PM7	12344.9498	72.1702	145.4274	-31014.2295
	PM6	12637.6310	74.4336	145.2024	-30654.4646
	PM6-DH2	12490.9828	73.8357	145.6349	-30930.0626
	RM1	12090.7567	71.3837	141.8785	-30210.3181
	PM3	12341.1070	71.8837	145.1935	-30948.3350
	AM1	12214.1290	70.2811	144.9420	-31000.3283
	MNDO	12243.8771	69.9765	145.6934	-31194.6101
Ammonia (1)	PM7	12537.7756	72.4852	146.5651	-31160.6090
	PM6	12590.5905	74.3477	143.8746	-30305.6215
	PM6-DH2	12528.3339	74.2562	143.6839	-30311.0209
	RM1	12330.7410	71.9632	145.7938	-31137.6805
	PM3	12204.5976	71.7935	144.2945	-30816.8076
	AM1	12188.8685	70.0350	145.0672	-31062.9172
	MNDO	11918.7039	69.3611	140.8084	-30063.3206
Dimethylformamide (1)	PM7	12562.6893	72.6695	146.3956	-31085.1588
	PM6	12821.3584	74.7295	148.0753	-31327.2923
	PM6-DH2	12580.3049	74.3054	144.3982	-30472.0184
	RM1	12372.3523	72.0518	143.2383	-30334.1468
	PM3	12170.7048	71.6367	143.6370	-30654.6668
	AM1	12075.6090	70.0062	142.6987	-30470.0084
	MNDO	12162.0476	69.7917	144.3621	-30879.5125
Acetonitrile (1)	PM7	12444.6038	72.2419	147.6490	-31576.9456
	PM6	12608.6123	74.4396	144.2081	-30387.0327
	PM6-DH2	12611.9997	74.4051	146.3983	-31036.6534
	RM1	12194.0458	71.5393	143.4879	-30586.8716
	PM3	12172.4318	71.6732	144.0373	-30772.2892
	AM1	11834.3396	69.1667	140.5481	-30070.0764
	MNDO	12132.4155	69.8185	142.9249	-30480.6434

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH, kcal/mol)	Heat capacity (C, cal/Kmol)	Entropy (ΔS, cal/Kmol)	Free Energy (ΔG, kcal/mol)
Methanol (2)	PM7	12929.5557	76.3485	148.2261	-31264.0560
	PM6	13339.6094	78.8770	149.9528	-31368.8179
	PM6-DH2	13241.0213	78.8255	147.5196	-30741.9474
	RM1	12941.9603	76.0338	149.2653	-31561.4889
	PM3	12688.9130	75.3796	146.3498	-30945.2799
	AM1	12833.7552	74.1173	148.3026	-31382.6650
	MNDO	12878.2383	73.7989	149.8486	-31799.1218
Ethanol (2)	PM7	13093.4780	76.8295	151.7552	-32152.3349
	PM6	13135.2049	78.4654	147.9217	-30967.6500
	PM6-DH2	13207.9813	78.7459	148.9360	-31197.2871
	RM1	12847.8330	75.5241	149.1062	-31608.1805
	PM3	12708.8774	75.5619	145.3660	-30631.9955
	AM1	12717.3942	73.8842	146.9269	-31088.8610
	MNDO	12719.6970	73.6627	146.8429	-31061.5136
Iso-Propyl Alcohol (2)	PM7	13028.7365	76.6499	148.8475	-31350.1456
	PM6	13259.5953	78.8124	147.3444	-30671.1376
	PM6-DH2	13189.8316	78.7441	146.9461	-30622.1481
	RM1	12863.8892	75.7351	147.5623	-31131.8105
	PM3	12780.0470	75.5327	149.8733	-31904.6774
	AM1	12694.2212	74.0078	149.0369	-31741.1305
	MNDO	12876.1747	73.9948	148.9772	-31541.3775
n-butyl alcohol (2)	PM7	12699.36030	75.4966	145.1213	-30568.5553
	PM6	13350.18410	78.7130	150.4945	-31519.7511
	PM6-DH2	13106.21700	78.3851	146.7610	-30650.5752
	RM1	12770.76990	75.3330	147.4428	-31189.3009
	PM3	12844.04040	75.6811	148.7541	-31506.9945
	AM1	12587.57510	73.6775	146.9326	-31220.3796
	MNDO	12876.45060	73.9438	149.4339	-31677.2667
tert-butyl alcohol (2)	PM7	12852.0857	76.1818	145.4008	-30499.1628
	PM6	13216.6901	78.6137	148.5562	-31075.3409
	PM6-DH2	13263.6141	78.4218	149.7415	-31381.8141
	RM1	12581.4056	74.9231	144.0747	-30374.4662
	PM3	12738.3263	75.5105	146.8975	-31059.1633
	AM1	12693.6041	73.7893	147.1616	-31182.6269
	MNDO	12833.9730	73.8082	150.0623	-31907.1017

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH, kcal/mol)	Heat capacity (C, cal/Kmol)	Entropy (ΔS, cal/Kmol)	Free Energy (ΔG, kcal/mol)
Ethylene glycol (2)	PM7	13040.2722	76.7691	149.3305	-31482.6164
	PM6	13388.9088	79.0436	151.7331	-31850.3150
	PM6-DH2	13364.9412	78.7168	152.8261	-32200.1605
	RM1	12815.4785	75.3668	149.2437	-31681.5307
	PM3	12668.6630	75.4063	146.4217	-30986.9669
	AM1	12632.2641	73.5649	146.5287	-31055.2678
	MNDO	12688.5545	73.5858	146.7997	-31079.7761
Dimetyl sulfoxide (2)	PM7	13000.1039	76.7086	149.5668	-31593.2375
	PM6	13384.8371	79.0599	151.3499	-31740.1356
	PM6-DH2	13330.0540	78.1720	153.2153	-32351.0877
	RM1	13099.8556	75.8624	154.4648	-32953.8245
	PM3	12728.0425	75.5074	148.7104	-31609.9633
	AM1	12628.5902	73.7504	147.5814	-31372.8042
	MNDO	12940.9044	74.0996	149.9209	-31758.0119
Ammonia (2)	PM7	12824.6068	76.0259	146.3272	-30802.8479
	PM6	13319.3326	79.0161	148.6837	-31010.7126
	PM6-DH2	13204.2950	78.4077	150.6502	-31712.0621
	RM1	12897.3779	76.0203	147.9384	-31210.4561
	PM3	12711.1127	75.5736	145.5644	-30688.9132
	AM1	12765.5621	73.9418	148.4394	-31491.6450
	MNDO	12952.4485	73.9578	151.3292	-32166.3525
Dimethylformamide (2)	PM7	13023.0418	76.7218	148.2544	-31179.0076
	PM6	13323.7461	78.4093	150.9754	-31689.5694
	PM6-DH2	13214.4158	77.9581	150.8497	-31761.4223
	RM1	13046.9517	75.9652	151.4463	-32106.7626
	PM3	12744.4928	75.4573	150.0810	-32002.1573
	AM1	12786.5916	74.0456	149.5910	-31813.9650
	MNDO	12978.2988	74.1772	150.2915	-31831.1119
Acetonitrile (2)	PM7	12814.4670	75.8416	146.5117	-30867.9964
	PM6	13177.4443	78.2919	149.1807	-31300.7814
	PM6-DH2	13319.3398	78.5599	152.1989	-32058.7622
	RM1	12884.2751	75.5922	149.6392	-31730.6524
	PM3	12620.3753	75.2127	145.7557	-30836.6867
	AM1	12576.8738	73.6551	146.7910	-31188.8629
	MNDO	12720.5374	73.7315	145.5542	-30676.4473

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH, kcal/mol)	Heat capacity (C, cal/Kmol)	Entropy (ΔS, cal/Kmol)	Free Energy (ΔG, kcal/mol)
Methanol (3)	PM7	13369.4116	76.5905	156.2155	-33206.2397
	PM6	13812.3299	78.9895	160.4526	-34026.6128
	PM6-DH2	13839.3833	79.0662	159.2062	-33627.9452
	RM1	13297.8339	76.1610	154.8880	-32882.0233
	PM3	13314.0075	76.4574	155.5654	-33067.8165
	AM1	13080.6337	74.2815	152.1971	-32296.9317
	MNDO	13259.1116	74.0833	157.4236	-33676.7347
Ethanol (3)	PM7	13421.1453	76.5633	161.2982	-34669.9160
	PM6	13603.7077	78.3446	156.5019	-33057.3338
	PM6-DH2	13756.6244	78.8044	158.9729	-33641.1457
	RM1	13166.0189	75.8895	152.6832	-32356.4772
	PM3	13378.6928	76.7129	155.0366	-32845.4695
	AM1	13088.2824	74.2554	151.9921	-32228.1622
	MNDO	13113.4195	73.9900	153.7812	-32736.4453
Iso-Propyl Alcohol (3)	PM7	13427.3726	76.6906	156.7747	-33315.0042
	PM6	13640.6110	78.6057	156.9199	-33145.0572
	PM6-DH2	13739.8621	78.8038	158.4306	-33496.2213
	RM1	13253.7429	76.1519	154.8546	-32916.1561
	PM3	13380.9246	76.6907	155.3558	-32938.4072
	AM1	12909.9495	73.9049	150.2237	-31879.2467
	MNDO	13267.8863	74.0953	157.6493	-33735.2525
n-butyl alcohol (3)	PM7	13441.0849	76.6503	156.9122	-33342.2875
	PM6	13799.7982	79.0607	159.9956	-33902.8899
	PM6-DH2	13746.3213	78.7508	159.8464	-33911.8829
	RM1	13183.2451	75.8831	152.8921	-32401.5345
	PM3	13154.7662	75.5600	157.4171	-33779.1422
	AM1	12951.5945	73.8978	151.4609	-32206.4728
	MNDO	13080.5627	73.8439	158.9803	-34319.4137
tert-butyl alcohol (3)	PM7	13431.7816	76.7440	155.1728	-32832.9887
	PM6	13789.6674	78.9760	158.8355	-33567.1369
	PM6-DH2	13526.8121	78.4992	154.3637	-32496.7251
	RM1	13110.2330	75.7655	151.5503	-32074.4889
	PM3	13376.1585	76.4850	156.7379	-33355.2464
	AM1	13092.7347	74.2223	153.4281	-32651.8533
	MNDO	13165.3698	74.0219	154.5372	-32909.8964

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH, kcal/mol)	Heat capacity (C, cal/Kmol)	Entropy (ΔS, cal/Kmol)	Free Energy (ΔG, kcal/mol)
Ethylene glycol (3)	PM7	13473.5690	76.8427	156.4227	-33163.8590
	PM6	13657.8929	78.6688	157.0164	-33156.5468
	PM6-DH2	13622.3879	78.6504	159.2607	-33861.1898
	RM1	13208.7037	75.9015	155.0513	-33019.8414
	PM3	13366.1309	76.5955	155.3947	-32964.7989
	AM1	13035.9566	74.1250	152.9506	-32566.2648
	MNDO	13317.0114	74.1287	158.5594	-33957.4737
Dimetyl sulfoxide (3)	PM7	13473.8879	76.8094	160.7134	-34442.8123
	PM6	13756.3918	78.8784	159.4814	-33792.9876
	PM6-DH2	13821.3998	79.0800	158.8575	-33541.9638
	RM1	13170.6978	75.9899	152.5078	-32299.5028
	PM3	13238.9418	76.0447	157.7132	-33783.2488
	AM1	13152.8399	74.3049	155.3705	-33170.8747
	MNDO	13246.7358	74.0818	157.1864	-33618.3894
Ammonia (3)	PM7	13400.4956	76.8779	155.9072	-33083.2361
	PM6	13615.1393	78.2972	159.2801	-33874.2225
	PM6-DH2	13731.3814	78.8686	160.7333	-34191.2520
	RM1	13528.8583	76.4716	159.3869	-33992.3459
	PM3	13364.8058	76.4916	156.5410	-33307.8934
	AM1	13044.1912	74.1421	152.0629	-32293.3624
	MNDO	12802.3660	73.2457	150.1216	-31956.3890
Dimethylformamide (3)	PM7	13282.2561	76.5257	153.1242	-32371.7241
	PM6	13526.5743	78.2070	155.7430	-32908.2012
	PM6-DH2	13524.1543	78.3746	154.2184	-32456.0617
	RM1	13137.5342	75.6966	153.6513	-32673.6009
	PM3	12682.2522	75.0393	148.0742	-31466.0705
	AM1	12988.9286	74.0118	151.8128	-32274.0577
	MNDO	13107.2273	73.9286	154.0240	-32815.0283
Acetonitrile (3)	PM7	13398.3534	76.5579	157.6548	-33606.4252
	PM6	13656.4072	78.7412	157.1380	-33194.2875
	PM6-DH2	13633.2416	78.5489	159.9601	-34058.8622
	RM1	13324.6182	76.2699	154.5778	-32762.7529
	PM3	13380.7679	76.5842	155.5031	-32982.4814
	AM1	13078.8454	74.0253	154.0973	-32865.2646
	MNDO	13227.6262	74.1567	155.1370	-33026.4704

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH. kcal/mol)	Heat capacity (C. cal/Kmol)	Entropy (ΔS. cal/Kmol)	Free Energy (ΔG. kcal/mol)
Methanol (4)	PM7	15627.7193	89.6065	170.6539	-35252.7410
	PM6	15967.1179	91.9145	175.0232	-36216.0492
	PM6-DH2	15812.3785	91.7419	170.7440	-35094.9451
	RM1	14916.1226	87.5901	166.3365	-34677.1049
	PM3	15739.1178	90.7702	173.1288	-35879.2339
	AM1	15367.4602	87.2515	170.9502	-35601.3419
	MNDO	15222.5687	86.3617	167.8313	-34816.3334
Ethanol (4)	PM7	15151.6819	88.4524	165.1107	-34076.0733
	PM6	15592.7447	91.4361	167.6018	-34377.7320
	PM6-DH2	15735.3046	91.5754	173.1075	-35876.6965
	RM1	15178.2711	87.9549	165.8872	-34280.9976
	PM3	15606.7982	90.2803	170.7556	-35303.9839
	AM1	15011.0251	86.6637	166.1850	-34537.0327
	MNDO	15168.2178	86.2479	167.1810	-34676.7974
Iso-Propyl Alcohol (4)	PM7	15506.7768	89.0535	170.8701	-35438.1435
	PM6	15760.3095	91.8939	169.5919	-34803.5155
	PM6-DH2	15913.6932	91.7310	171.4214	-35195.5972
	RM1	15123.8380	87.5745	168.3546	-35071.0860
	PM3	15811.0678	90.9824	171.1031	-35203.3215
	AM1	14916.9269	86.6943	162.7776	-33615.2145
	MNDO	15058.4256	86.2020	165.7043	-34346.3114
n-butyl alcohol (4)	PM7	15491.1949	88.7179	171.8462	-35744.7496
	PM6	15827.0832	91.5367	174.8976	-36318.6362
	PM6-DH2	15143.8275	89.4367	164.8666	-34011.1493
	RM1	14817.2945	86.8788	164.8763	-34340.5743
	PM3	15533.1110	90.4953	168.3645	-34664.7647
	AM1	14941.6457	86.5109	163.3612	-33764.4961
	MNDO	15079.1370	86.1519	166.8003	-34652.3724
tert-butyl alcohol (4)	PM7	15556.4660	89.4218	168.7992	-34771.0155
	PM6	15621.7573	91.1916	172.3435	-35762.4572
	PM6-DH2	15687.8251	90.4159	171.4994	-35444.7210
	RM1	14862.5570	87.5989	161.8630	-33396.8965
	PM3	15612.3453	90.2969	175.4622	-36701.7096
	AM1	15104.6906	86.7799	168.7905	-35220.1970
	MNDO	14913.5149	85.5566	165.9209	-34555.8014

Solvent (Molecule)	Method	Thermodynamic Properties			
		Enthalpy (ΔH. kcal/mol)	Heat capacity (C. cal/Kmol)	Entropy (ΔS. cal/Kmol)	Free Energy (ΔG. kcal/mol)
Ethylene glycol (4)	PM7	15526.1915	89.2531	169.1319	-34900.4845
	PM6	15470.5264	90.9538	173.7343	-36328.3551
	PM6-DH2	15542.4528	90.8494	168.2475	-34620.5393
	RM1	15097.5639	88.0608	164.2147	-33863.0489
	PM3	15641.8817	90.7374	168.3964	-34565.5050
	AM1	15192.8416	87.0708	167.4790	-34741.0223
	MNDO	14925.8394	85.8484	163.8859	-33936.7417
Dimetyl sulfoxide (4)	PM7	15733.8288	89.6561	172.8718	-35807.8984
	PM6	15797.8184	91.8854	169.7797	-34821.9992
	PM6-DH2	15784.5639	91.5686	170.2812	-34984.7759
	RM1	14803.6320	86.9723	161.7543	-33423.4125
	PM3	15387.7508	90.3324	165.2525	-33882.2821
	AM1	14772.0342	86.1190	159.7442	-32855.6990
	MNDO	15222.4385	86.2792	168.7729	-35097.2016
Ammonia (4)	PM7	15604.0156	89.5177	169.5684	-34952.8029
	PM6	15698.0564	91.5050	171.1586	-35332.8802
	PM6-DH2	15595.5430	91.1629	169.4481	-34925.4080
	RM1	14963.0918	87.4058	164.1704	-33984.3130
	PM3	15532.7781	90.2532	168.9037	-34825.8601
	AM1	14894.6236	86.4277	165.3518	-34405.0156
	MNDO	15222.9217	86.3588	166.3269	-34367.4435
Dimethylformamide (4)	PM7	15754.2843	89.7260	173.2155	-35889.9170
	PM6	15632.4693	91.3973	169.7314	-34972.9476
	PM6-DH2	15802.9640	91.7539	169.9688	-34873.2337
	RM1	14789.0119	87.2154	160.4519	-33049.7221
	PM3	15629.6805	90.5574	170.2516	-35130.8340
	AM1	14828.6029	86.1029	164.0306	-34077.1205
	MNDO	14826.4711	85.0572	164.0565	-34086.9744
Acetonitrile (4)	PM7	15580.5269	89.5726	173.0758	-36022.0229
	PM6	15043.5241	89.9988	164.1488	-33897.4406
	PM6-DH2	15641.2712	91.4131	170.1464	-35087.8780
	RM1	15138.3255	87.9891	166.9427	-34635.6405
	PM3	15393.3919	89.6917	169.1885	-35050.1594
	AM1	15153.5211	86.8659	168.4563	-35071.7247
	MNDO	14870.0703	85.5470	163.2009	-33788.2780

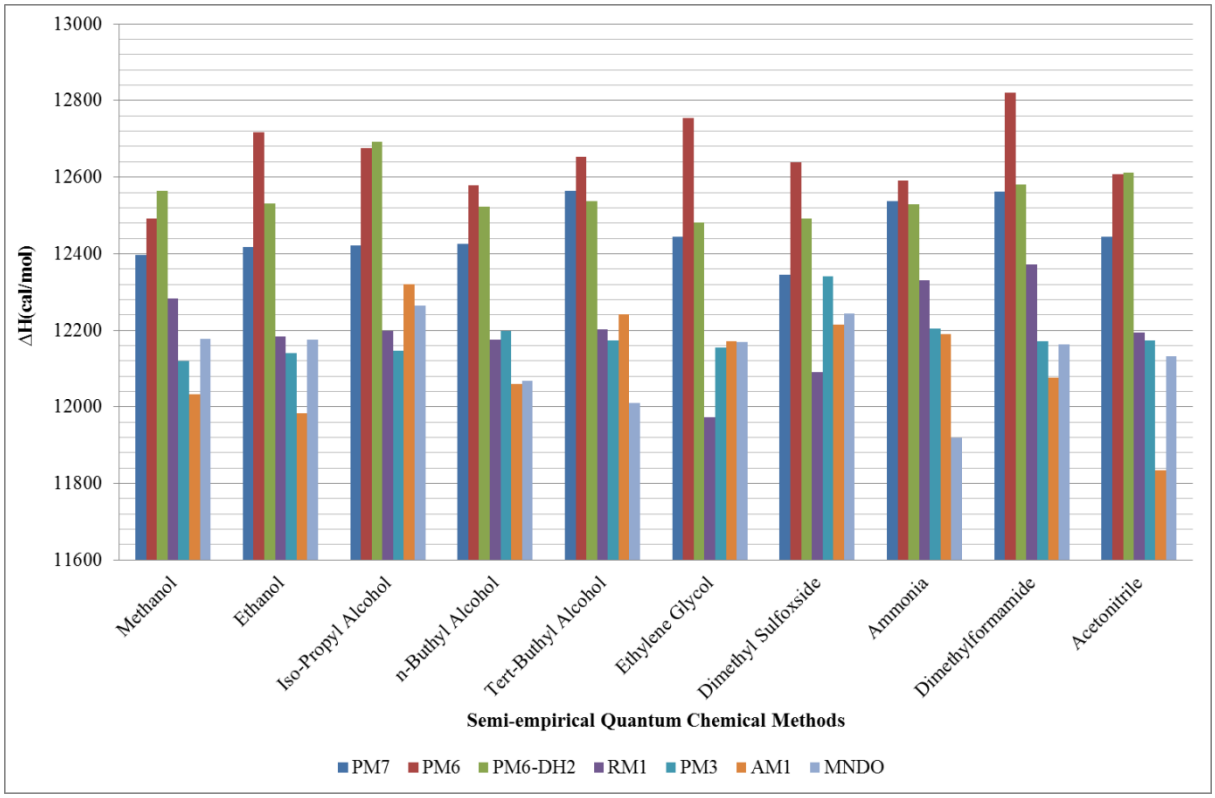


Fig. 1: The change in enthalpy for the 1. molecule in working solvent media

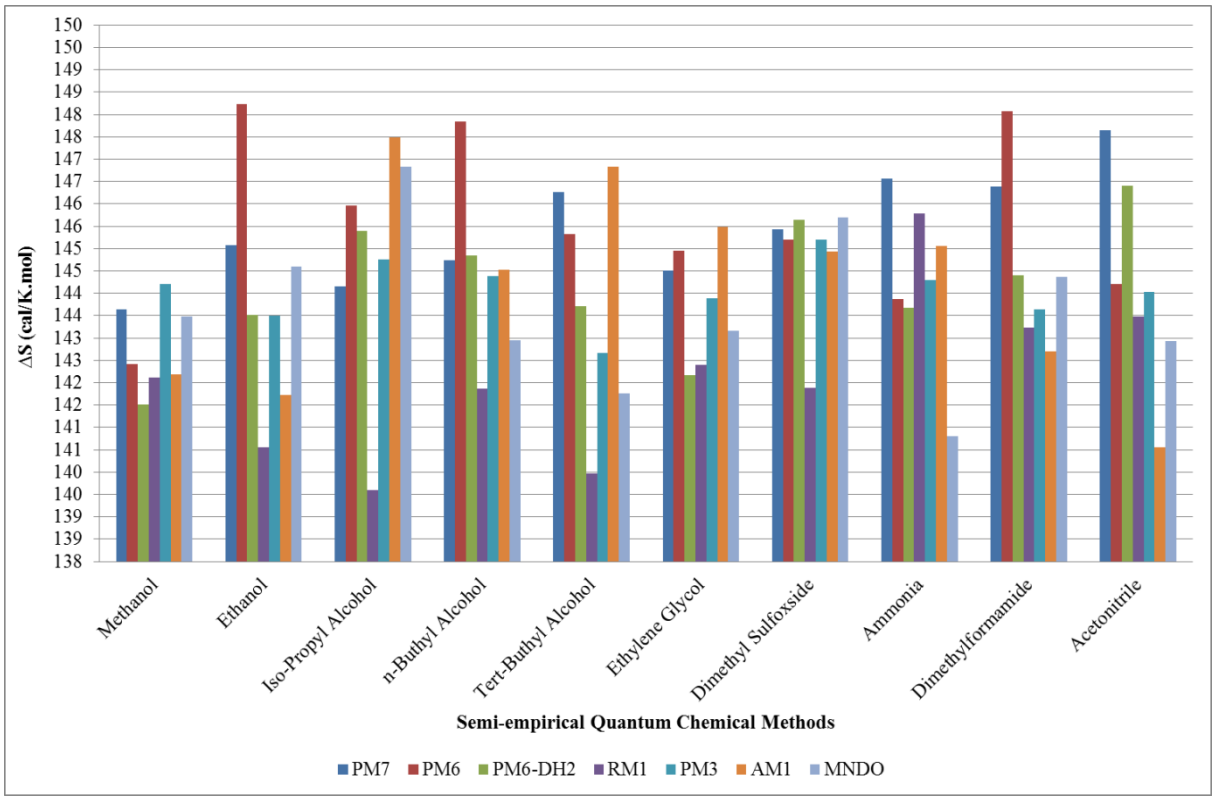


Fig. 2: The change in entropy for the 1. molecule in working solvent media

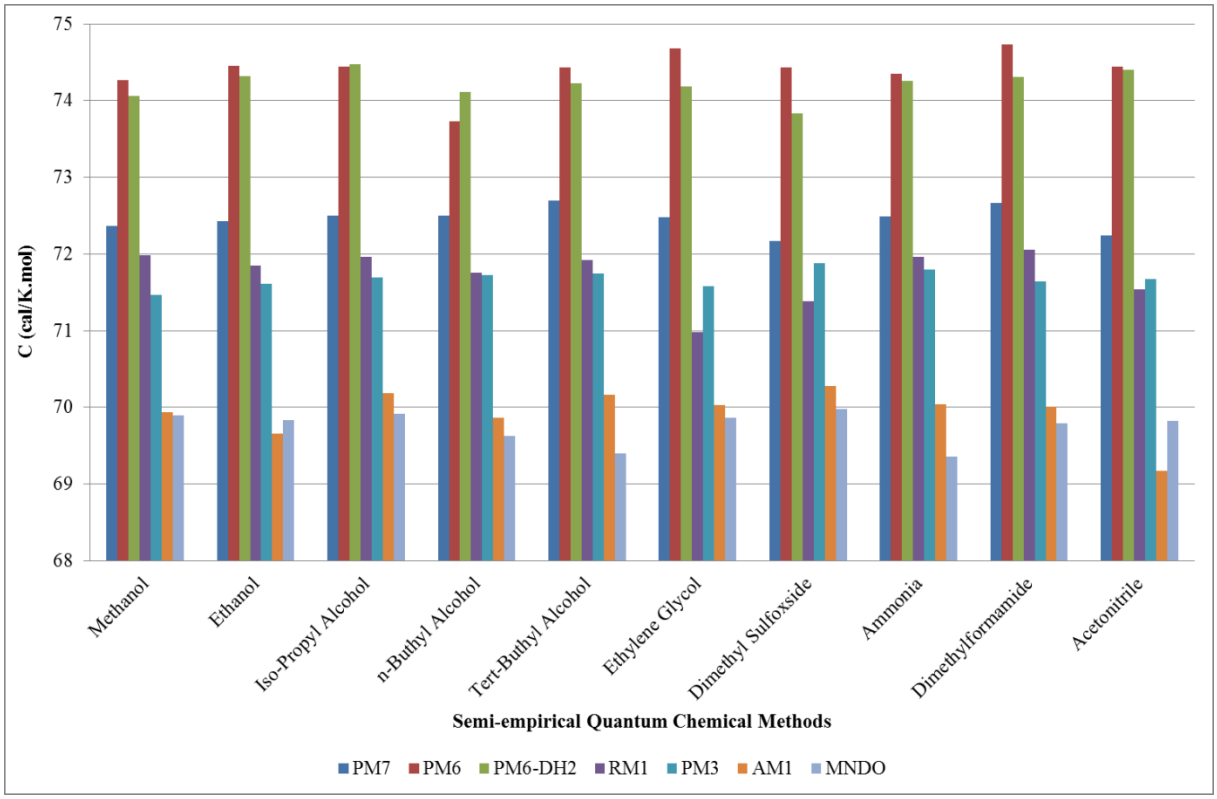


Fig. 3: The change in heat capacity for the 1. molecule in working solvent media

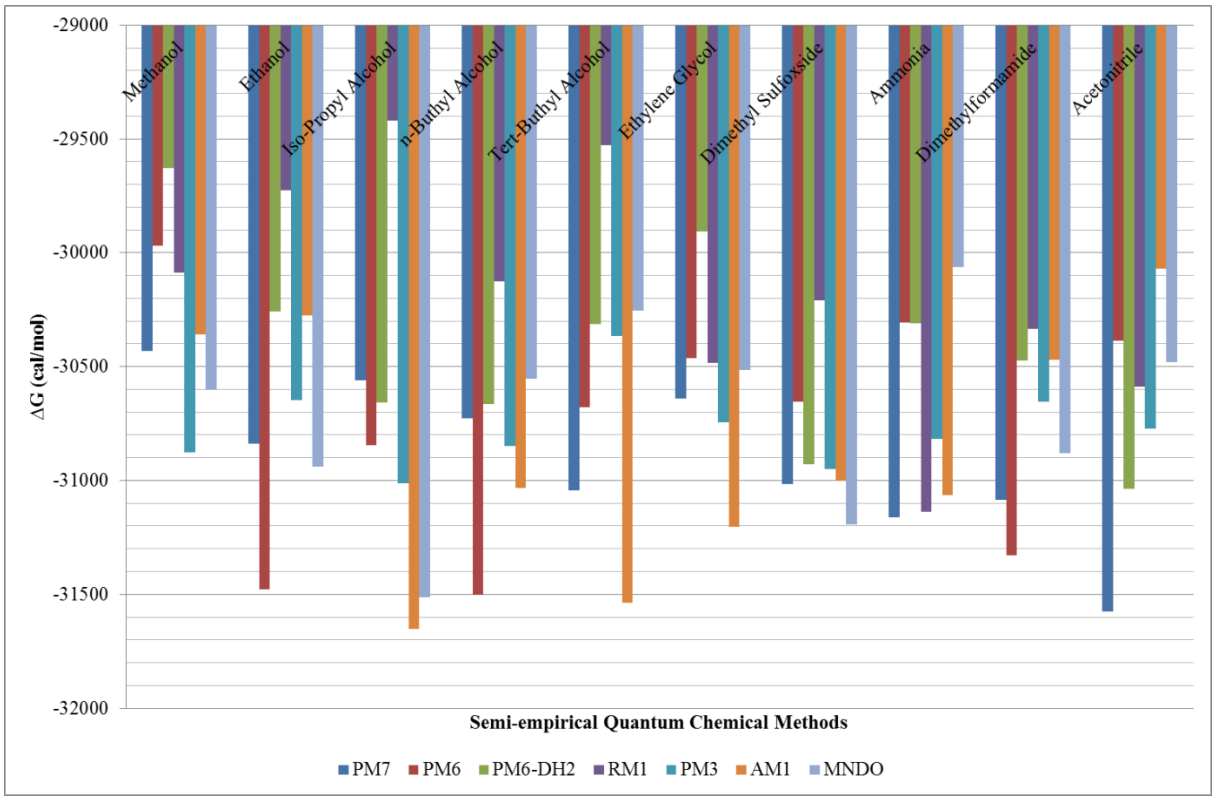


Fig. 4: The change in free energy for the 1. molecule in working solvent media

When the results are analyzed, the highest enthalpy value of 4th molecule was determined as 15967.1179 cal/mol with PM6 model in methanol media and the lowest enthalpy value of 1st molecule was determined as 11834.3396 cal/mol with with AM1 model in acetonitrile media. The highest entropy value of 4th molecule was determined as 175.4622 cal/K.mol with PM3 model in tert-buthyl alcohol media and the lowest enthalpy value of 1st molecule was determined as 139.5945 cal/K.mol with with RM1 model in iso-prophyl alcohol media. The highest heat capacity value of 4th molecule was determined as 91.9145 cal/K.mol with PM6 model in methanol media and the lowest heat capacity value of 1st molecule was determined as 69.1667 cal/K.mol with with AM1 model in acetonitrile media. Finally, the highest free energy value of 4th molecule was determined as 36701.7096 cal/mol with PM3 model in tert-buthyl alcohol media and the lowest free energy value of 1st molecule was determined as 29421.2024 cal/mol with with RM1 model in iso-prophyl alcohol media. Graphical representation of the values mentioned here are given Figure 5 – 8.

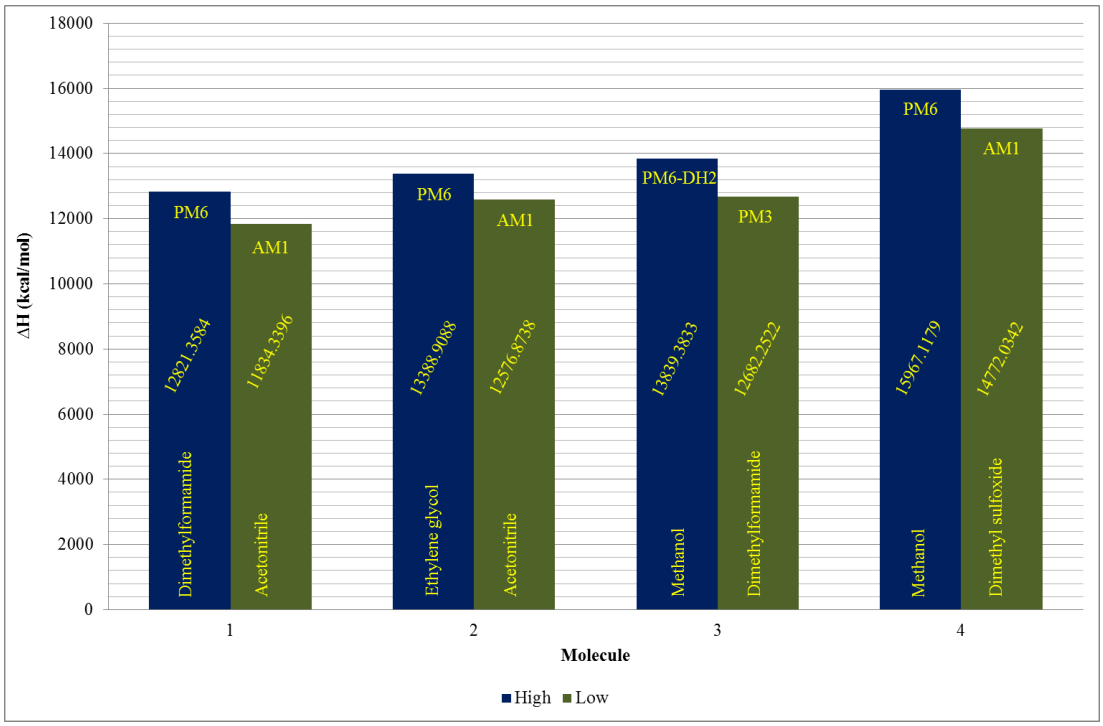


Fig. 5: The change of the highest and the lowest enthalpy values for working molecules

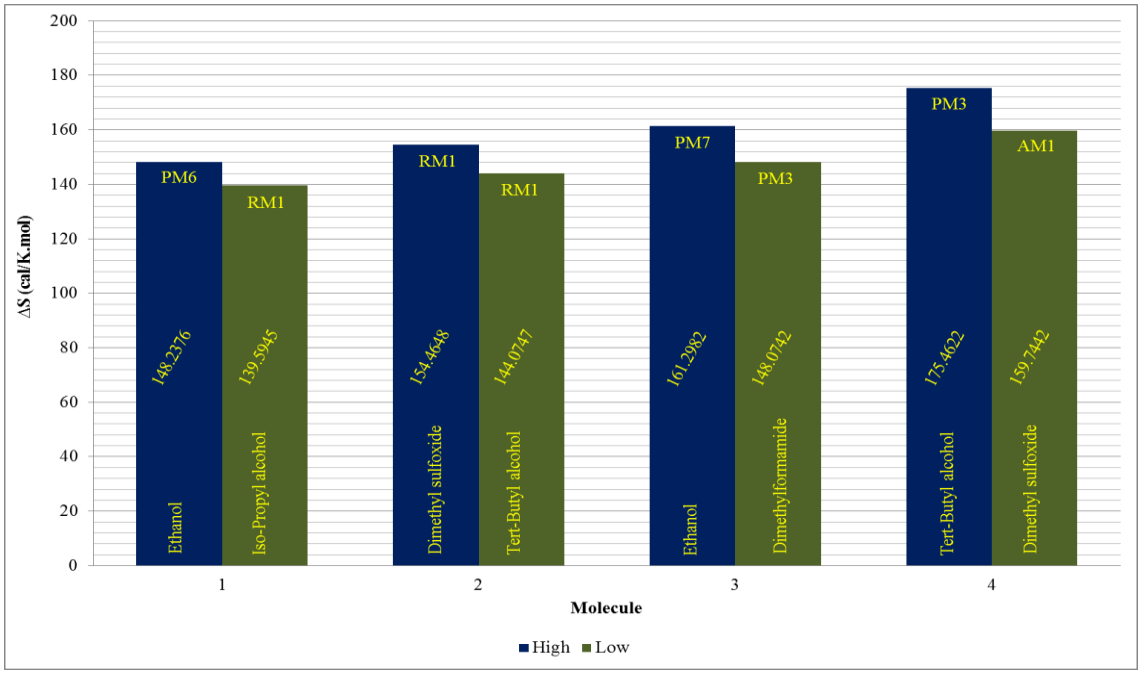


Fig. 6: The change of the highest and the lowest entropy values for working molecules

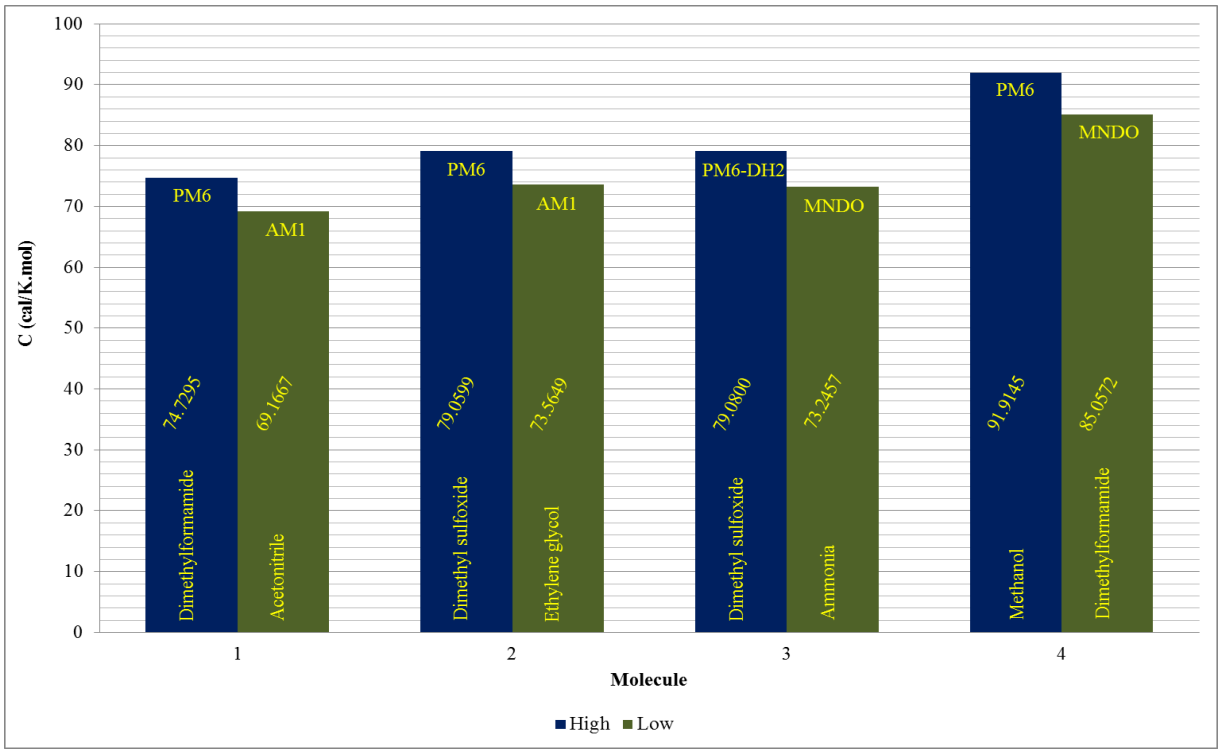


Fig. 7: The change of the highest and the lowest heat capacity values for working molecules

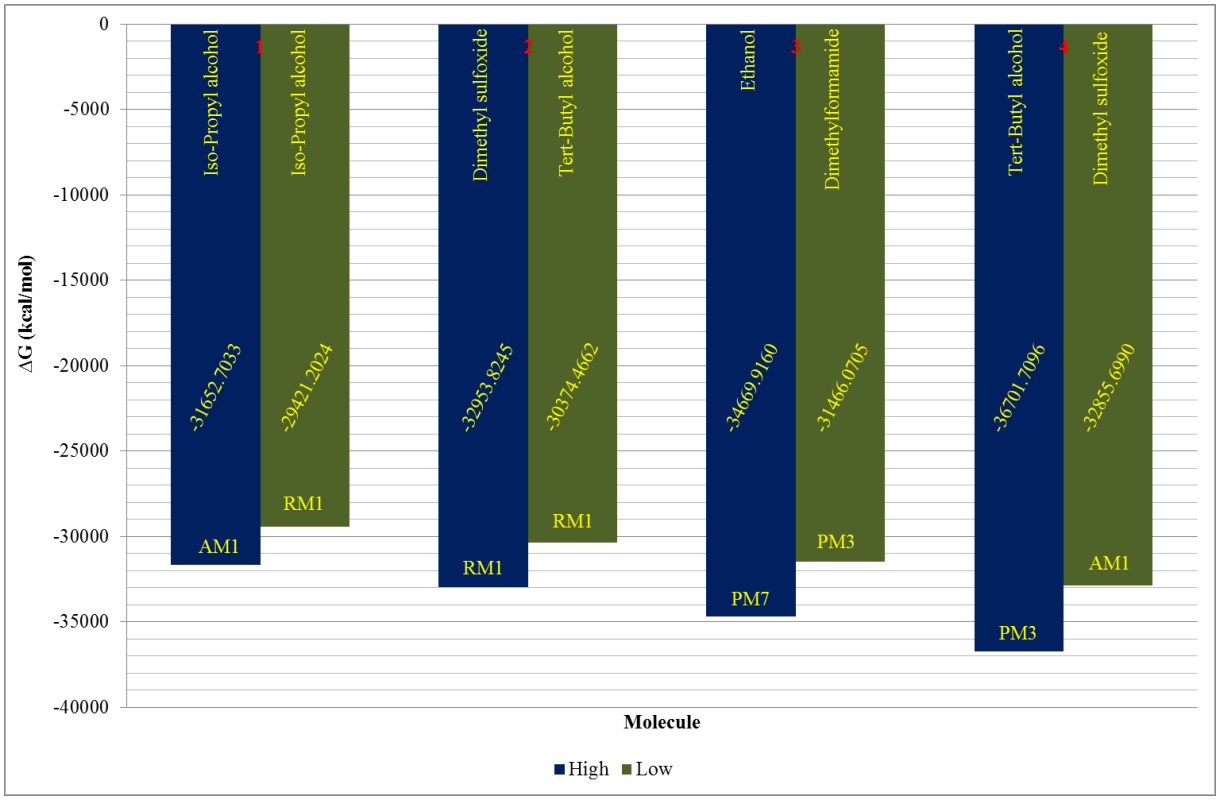


Fig. 8: The change of the highest and the lowest free energy values for working molecules

CONCLUSION

As a result, studied these four some eugenol derivatives were calculated some of the important thermodynamic properties (enthalpy (ΔH, kcal/mol), heat capacity (C, cal/Kmol), entropy (ΔS, cal/Kmol) and free energy (ΔG, kcal/mol)) using semi-empirical quantum chemical methods (PM7, PM6, PM6-DH2, RM1, PM3, AM1 and MNDO) with the MOPAC 2016 computer program in different solvents (methyl alcohol, ethyl alcohol, isopropyl alcohol, n-butyl alcohol, tert-butyl alcohol, ethylene glycol, dimetyl sulfoxide, ammonia, N,N-dimethyl formamide and acetonitrile) at 298 K. These values will provide significant contributions at the point of use in many processes.

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