

An Extensive Theoretical Study on the Thermochemistry of Aromatic Compounds: From Electronic Structure to Group Additivity Values

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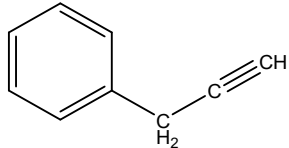
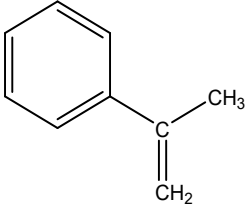
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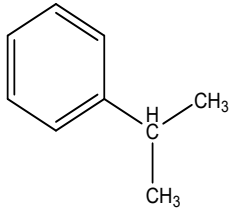
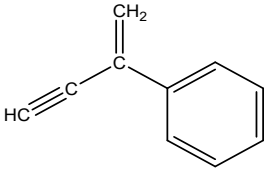
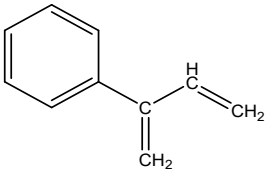
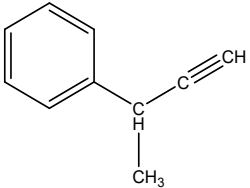
Supporting Information

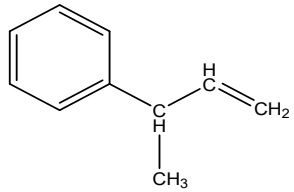
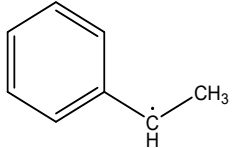
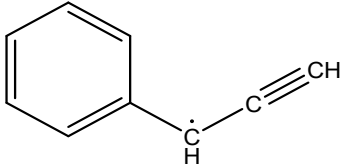
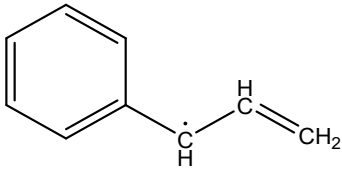
Table S1 0 K enthalpies of formation for reference species in isodesmic reactions from ATcT (kcal/mol)

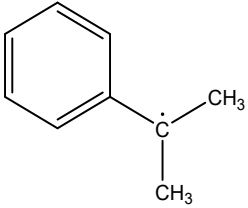
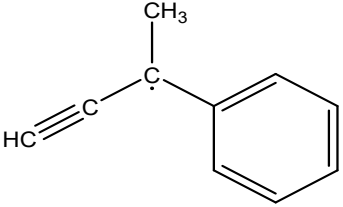
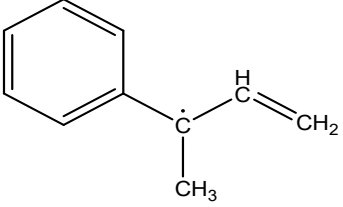
Species	$\Delta H_f(0K)$	Species	$\Delta H_f(0K)$
Anisole	-11.42	Propylene	8.34
Styrene	40.53	Ethylene	14.54
Methylbenzene	17.51	Ethane	-16.33
Formic acid	-88.66	Methane	-15.90
Methanol	-45.39		

Table S 2 Thermochemistry comparison of monosubstituted aromatics against Sabbe et al.

Species	Resource	$\Delta H_f(298.15\text{K})$ [kcal/mol]	$S(298.15\text{K})$ [cal/mol/K]	C_p [cal/mol/K]						
				300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
 3-phenyl-1-propyne	This work	72.9	89.1	31.9	41.3	49.5	56.2	65.7	72.6	82.6
	Sabbe et al.	73.5	88.8	31.8	41.5	49.5	56.1	65.8	72.6	
 alpha-methyl-styrene	This work	27.8	90.1	34.1	44.3	53.3	60.9	71.7	79.6	91.3
	Sabbe et al.	27.9	90.3	33.9	44.4	53.3	60.7	71.7	79.5	
 3-phenylpropene	This work	32.1	93.0	33.6	43.9	53.1	60.8	71.7	79.6	91.3
	Sabbe et al.	32.5	93.2	33.7	44.2	53.2	60.6	71.7	79.5	

 <p>2-phenylpropane</p>	This work	0.3	93.1	36.3	47.4	57.4	65.8	77.9	86.7	100.0
	Sabbe et al.	0.7	92.3	36.6	47.9	57.7	65.8	78.0	86.7	
 <p>3-phenyl-3-buten-1-yne</p>	This work	92.1	92.6	35.7	45.9	54.6	61.6	71.4	78.3	88.5
	Sabbe et al.	92.7	92.8	35.9	46.3	54.9	61.6	71.4	78.2	
 <p>2-phenyl-1,3-butadiene</p>	This work	50.5	95.5	38.7	49.6	59.0	66.8	77.7	85.6	97.2
	Sabbe et al.	50.8	93.5	38.5	50.0	59.4	66.9	77.9	85.6	
 <p>3-phenyl-1-butyne</p>	This work	66.1	97.0	38.7	49.4	58.7	66.4	77.3	85.2	97.0

	Sabbe et al.	66.8	97.1	38.7	49.7	58.8	66.3	77.3	85.2	
 3-phenyl-1-butene	This work	25.8	100.7	39.9	51.3	61.7	70.5	83.0	92.1	105.6
	Sabbe et al.	26.1	102.2	39.0	51.0	61.3	69.8	82.6	91.6	
 1-phenyl-1-ethyl	This work	42.7	85.6	30.1	39.4	47.7	54.7	64.6	71.8	82.2
	Sabbe et al.	43.7	85.8	29.8	39.3	47.5	54.2	64.3	71.4	
 3-phenyl-1-propyn-3-yl	This work	100.8	87.3	32.4	41.6	49.3	55.6	64.3	70.5	79.3
	Sabbe et al.	101.5	87.7	32.7	41.9	49.5	55.4	64.2	70.2	
 3-phenyl-1-propen-3-yl	This work	58.8	88.7	33.9	44.6	53.9	61.5	71.7	78.8	88.8

	Sabbe et al.	59.3	88.8	33.4	43.9	52.7	59.8	70.3	77.7	
 2-phenyl-2-propyl	This work	35.6	93.4	35.0	45.4	55.0	63.1	74.9	83.4	95.9
	Sabbe et al.	35.9	93.8	34.4	45.2	54.8	62.6	74.6	83.1	
 3-phenyl-1-butyn-3-yl	This work	92.9	95.8	38.0	48.2	57.0	64.4	74.9	82.3	93.2
	Sabbe et al.	93.8	96.1	38.0	48.4	57.0	64.1	74.6	82.1	
 3-phenyl-1-buten-3-yl	This work	53.0	98.1	38.8	50.4	60.7	69.2	81.3	89.8	102.2
	Sabbe et al.	53.2	96.2	38.3	50.0	60.2	68.4	80.7	89.4	

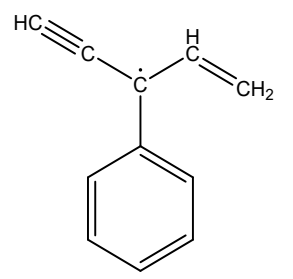
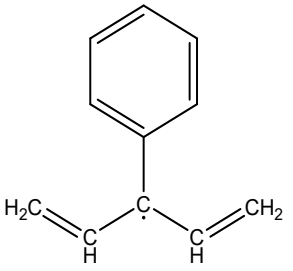
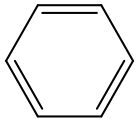
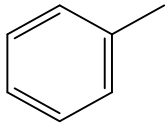
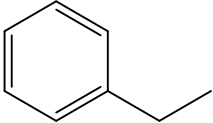
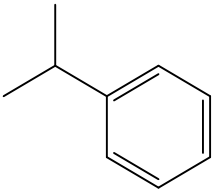
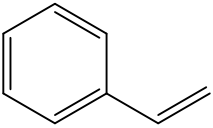
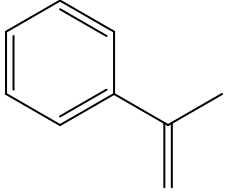
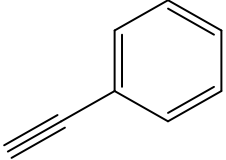
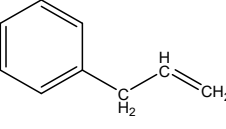
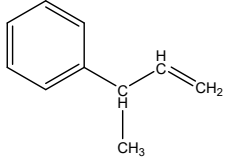
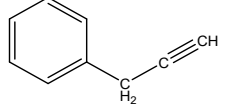
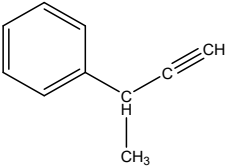
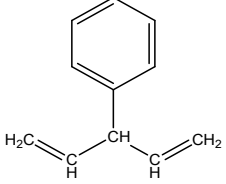
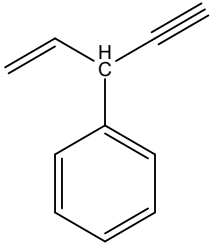
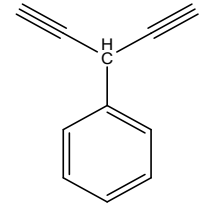
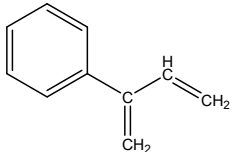
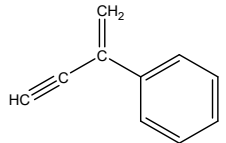
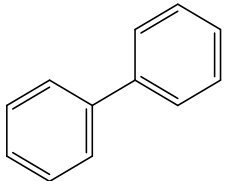
 3-phenyl-1-penten-4-yn-3-yl	This work	112.2	99.7	41.3	53.0	62.8	70.6	81.2	88.7	99.4
	Sabbe et al.	113.0	100.0	41.1	52.6	62.0	69.6	80.6	88.3	
 3-phenyl-1,4-pentadien-3-yl	This work	72.8	101.5	44.4	56.9	67.7	76.4	88.2	96.6	108.5
	Sabbe et al.	75.4	98.5	41.8	54.6	65.4	74.1	86.8	95.8	

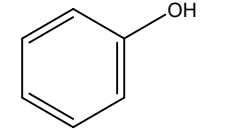
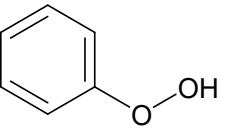
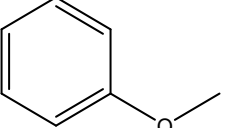
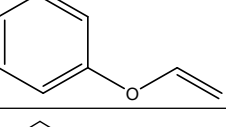
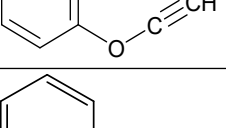
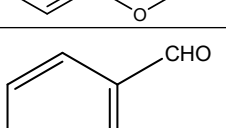
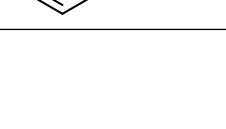
Table S 3 Thermochemistry of monosubstituted aromatics.

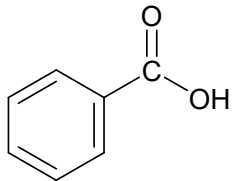
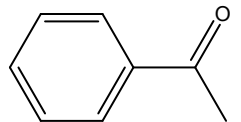
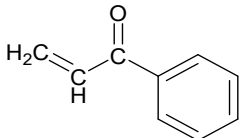
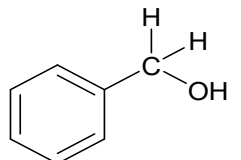
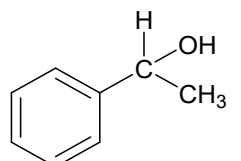
No.	Species	σ_{ext}	σ_{int}	n_{opt}	$\Delta H_f(298.15\text{K})$ [kcal/mol]	$S(298.15\text{K})$ [cal/mol/K]	C_p [cal/mol/K]					
							300 K	400 K	500 K	600 K	800 K	1000 K

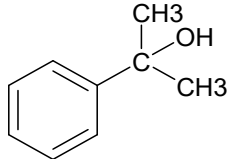
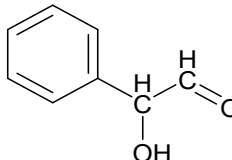
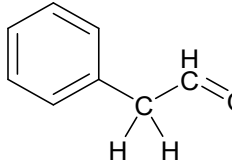
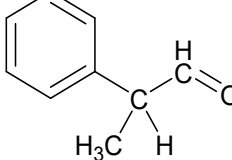
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3		1	6	1	6.9	86.3	30.3	39.9	48.6	56.1	66.6	74.3	85.7
4		1	18	1	0.3	93.1	36.3	47.4	57.4	65.8	77.9	86.7	100.0
5		1	2	1	35.4	82.0	28.3	37.4	45.4	52.1	61.3	67.8	77.4
6		1	6	1	27.8	90.1	34.1	44.3	53.3	60.9	71.7	79.6	91.2

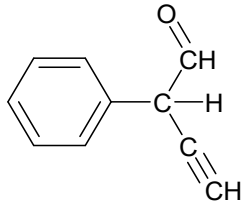
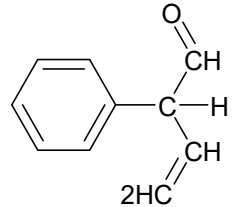
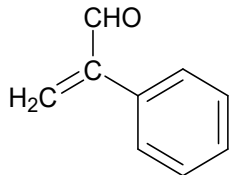
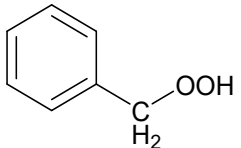
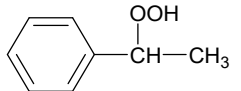
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8		1	2	1	32.1	93.0	33.6	43.9	53.1	60.8	71.7	79.6	91.3
9		1	6	2	25.8	100.7	39.9	51.3	61.7	70.5	83.0	92.1	105.6
10		1	2	1	72.9	89.1	31.9	41.3	49.5	56.2	65.8	72.6	82.6
11		1	6	2	66.1	97.0	38.7	49.4	58.7	66.4	77.3	85.2	97.0
12		1	2	1	51.5	109.7	44.7	56.5	66.9	75.7	88.3	97.5	111.2

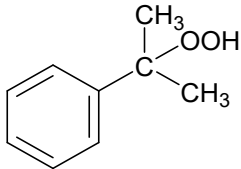
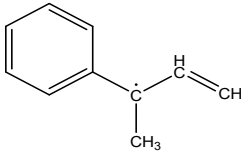
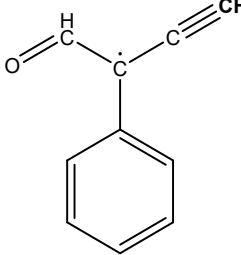
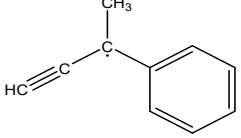
13		1	2	2	92.1	103.7	41.5	53.0	62.8	70.9	82.2	90.4	102.5
14		1	2	1	136.4	99.3	39.2	49.8	58.7	66.0	76.0	83.2	93.8
15		1	2	1	50.5	95.5	38.7	49.6	59.0	66.8	77.7	85.6	97.2
16		1	2	1	92.1	92.6	35.7	45.9	54.6	61.6	71.4	78.3	88.5
17		4	2	1	42.1	92.7	39.3	52.5	64.0	73.5	86.5	95.6	108.7

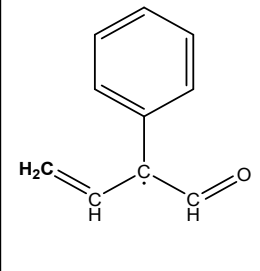
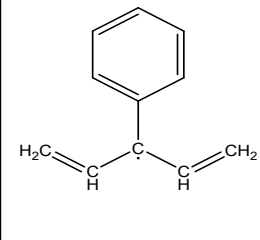
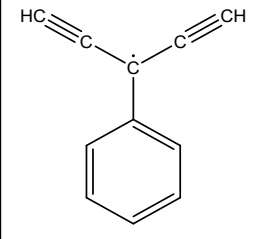
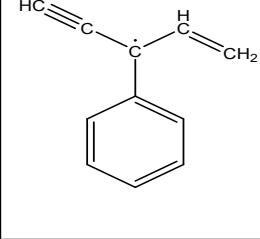
18		1	2	1	-21.9	75.2	24.8	32.2	38.5	43.5	50.4	55.3	62.4
19		1	2	2	-0.1	86.3	27.9	35.4	42.0	47.4	54.8	60.0	67.4
20		1	6	1	-17.1	82.5	29.4	38.1	45.8	52.1	60.9	67.3	76.6
21		1	2	1	4.4	91.1	31.9	41.2	49.4	56.1	65.5	72.2	82.0
22		1	2	1	56.0	85.7	31.4	40.1	47.2	52.9	60.6	66.0	73.8
23		1	2	1	-53.3	88.1	29.4	38.1	45.7	52.0	60.4	66.1	73.9
24		1	2	1	-9.2	79.5	26.4	34.2	41.1	46.9	55.1	60.8	68.8

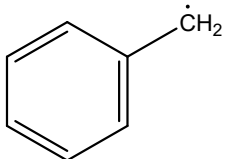
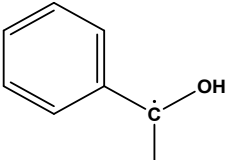
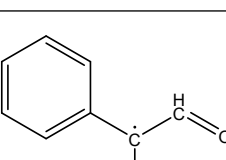
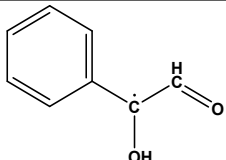
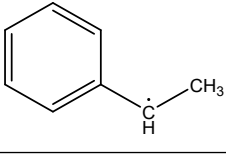
25		1	2	1	-71.0	84.5	29.9	38.5	46.0	52.2	60.9	67.2	75.6
26		1	6	1	-20.2	87.9	32.3	41.4	49.5	56.3	65.9	72.7	82.6
27		1	2	1	5.9	93.3	35.3	45.6	54.4	61.7	71.7	78.6	88.5
28		1	2	1	-22.7	86.4	29.6	37.9	45.3	51.5	60.3	66.7	76.2
29		1	6	2	-32.6	93.7	36.9	46.5	54.9	61.9	72.1	79.5	90.6

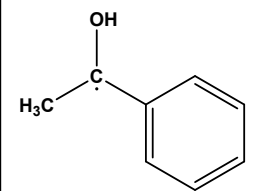
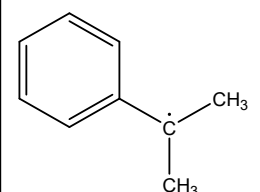
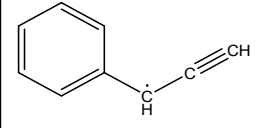
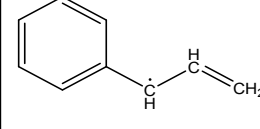
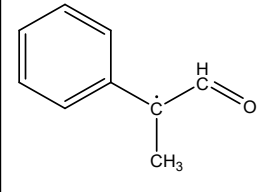
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31		1	2	2	-51.9	95.4	36.4	47.2	56.6	64.1	73.7	80.0	88.6
32		1	2	1	-12.1	92.7	30.6	39.8	48.1	55.1	64.8	71.8	81.9
33		1	6	2	-19.2	98.9	39.0	49.3	58.2	65.6	76.6	84.5	96.3

34		1	2	2	48.4	102.0	40.7	50.8	59.4	66.3	76.2	83.2	93.4
35		1	2	2	7.3	105.3	42.7	53.5	62.9	70.8	82.0	90.1	102.0
36		1	2	1	7.7	94.2	35.8	45.5	54.1	61.2	71.3	78.3	88.4
37		1	2	2	-5.5	95.7	33.2	42.0	49.8	56.4	65.6	72.1	81.6
38		1	6	4	-15.4	102.4	40.7	50.7	59.6	67.1	77.6	85.1	96.2

39		1	18	2	-24.1	106.4	47.6	59.5	69.7	78.1	89.8	98.3	110.8
40		1	6	1	53.0	98.1	38.8	50.4	60.7	69.2	81.3	89.8	102.1
41		1	2	1	71.6	99.1	38.7	49.0	57.7	64.8	74.5	81.2	90.4
42		1	6	1	92.9	95.8	38.0	48.2	57.0	64.4	74.9	82.4	93.2

43		1	2	1	33.4	102.0	41.1	52.1	61.6	69.6	80.7	88.4	99.3
44		2	2	1	72.8	101.5	44.4	56.9	67.7	76.4	88.2	96.6	108.5
45		2	2	1	154.9	96.7	40.0	50.1	58.5	65.1	74.4	80.9	90.3
46		1	2	1	112.2	99.7	41.3	53.0	62.8	70.6	81.2	88.7	99.4

47		2	2	1	50.2	75.7	25.8	33.8	40.8	46.5	54.4	60.0	68.2
48		1	2	1	8.8	84.2	30.0	38.3	45.4	51.2	59.1	64.8	73.0
49		1	2	1	19.3	88.0	31.6	40.7	48.5	55.0	64.1	70.4	79.3
50		1	2	1	-31.9	92.6	34.5	44.2	52.7	59.7	69.8	76.9	86.8
51		1	6	1	42.7	85.6	30.1	39.4	47.7	54.7	64.6	71.8	82.2

52		1	6	1	-0.7	93.9	34.2	43.9	52.4	59.4	69.3	76.4	86.9
53		2	18	1	35.6	93.4	35.0	45.4	55.0	63.1	74.9	83.4	95.9
54		1	2	1	100.8	87.3	32.4	41.6	49.3	55.6	64.3	70.5	79.3
55		1	2	1	58.8	88.7	33.9	44.6	53.9	61.5	71.7	78.8	88.8
56		1	6	1	11.4	97.4	36.4	46.6	55.6	63.3	74.1	81.8	92.9

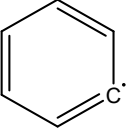
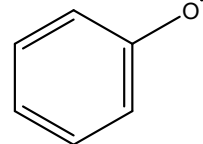
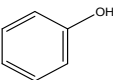
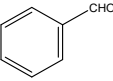
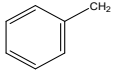
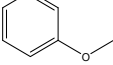
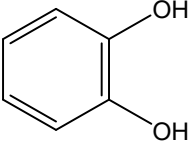
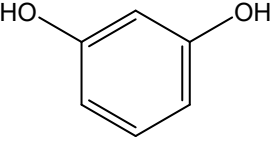
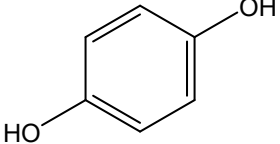
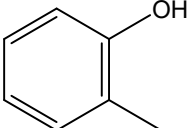
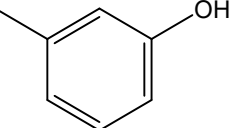
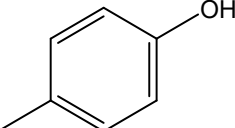
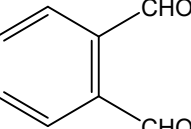
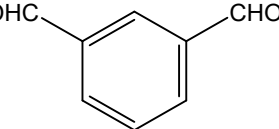
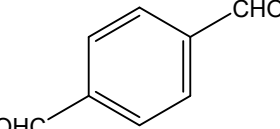
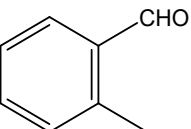
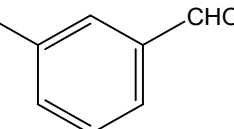
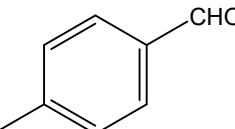
57		2	none	1	81.5	68.9	19.1	25.5	31.1	35.8	42.1	46.6	53.0
58		2	none	1	13.8	74.2	23.0	29.9	35.9	40.8	47.5	52.1	58.8

Table S 4 Thermochemistry comparison with hindered rotor potentials calculated at M06-X/6-31G and M06-X/6-311++G(d,p) level of theory.

Species	Methods	$\Delta H_f(298.15\text{K})$ [kcal/mol]	$S(298.15\text{K})$ [cal/mol/K]	C_p [cal/mol/K]						
				300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
 Phenol	M06-X/6-31G	-21.94	75.19	24.80	32.19	38.47	43.53	50.43	55.29	62.42
	M06-X/6-311++G(d,p)	-21.92	75.33	24.81	32.14	38.38	43.42	50.33	55.21	62.38
 Benzaldehyde	M06-X/6-31G	-9.20	79.49	26.36	34.17	41.12	46.92	55.08	60.80	68.82
	M06-X/6-311++G(d,p)	-9.18	79.70	26.37	34.19	41.15	46.95	55.08	60.75	68.68
 Benzyl radical	M06-X/6-31G	50.18	75.72	25.81	33.84	40.78	46.47	54.39	60.04	68.24
	M06-X/6-311++G(d,p)	50.18	75.75	25.83	33.85	40.79	46.47	54.39	60.04	68.22
 Anisole	M06-X/6-31G	-17.13	82.49	29.42	38.14	45.78	52.10	60.92	67.26	76.60

Anisole	M06-X/6-311++G(d,p)	-17.14	82.46	29.41	38.14	45.78	52.10	60.93	67.28	76.63
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Table S 5 The total symmetry number ($\sigma_{\text{total sysm}}$) and optical isomer number (n_{opt}) of disubstituted aromatics

Species	σ_{ext}	σ_{int}	n_{opt}	Species	σ_{ext}	σ_{int}	n_{opt}	Species	σ_{ext}	σ_{int}	n_{opt}
 O-dihydroxybenzene	2	1	1	 M-dihydroxybenzene	2	1	1	 P-dihydroxybenzene	4	1	1
 O-methylphenol	1	3	1	 M-methylphenol	1	3	1	 P-methylphenol	2	3	1
 O-phthalaldehyde	2	1	1	 M-phthalaldehyde	2	1	1	 P-phthalaldehyde	4	1	1
 O-methylbenzaldehyde	1	3	1	 M-methylbenzaldehyde	1	3	1	 P-methylbenzaldehyde	1	3	1

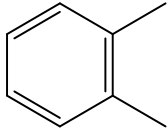
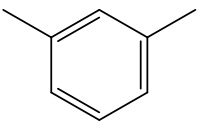
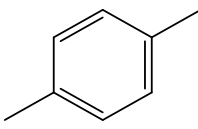
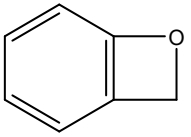
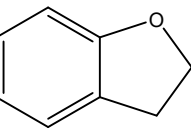
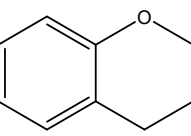
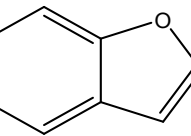
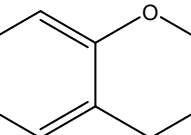
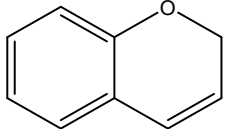
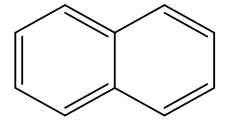
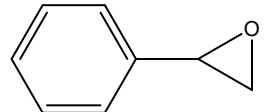
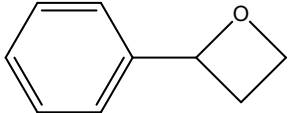
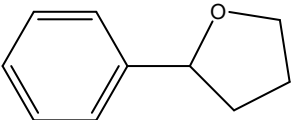
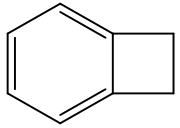
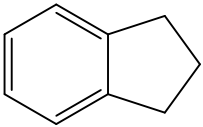
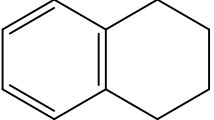
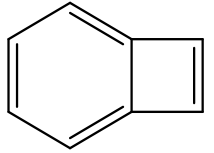
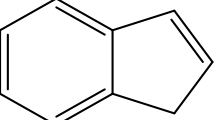
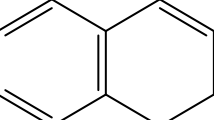
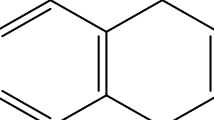
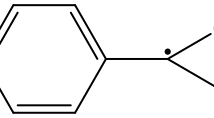
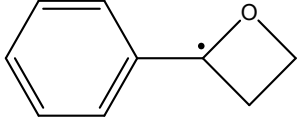
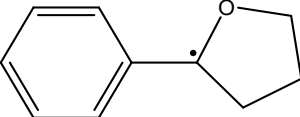
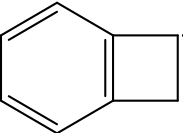
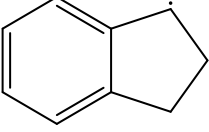
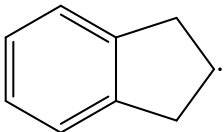
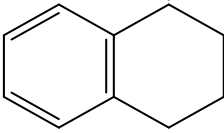
O-methylbenzaldehyde				M-methylbenzaldehyde				P-methylbenzaldehyde			
 O-xylene	2	9	1	 M-xylene	2	9	1	 P-xylene	4	9	1

Table S 6 Thermochemistry of dicyclic aromatics.

No.	Species	σ_{ext}	σ_{int}	n_{opt}	$\Delta H_f(298.15\text{K})$ [kcal/mol]	$S(298.15\text{K})$ [cal/mol/K]	C_p [cal/mol/K]						
							300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
59		1	none	1	23.3	76.2	25.1	33.3	40.6	46.6	54.9	60.6	68.8
60		1	none	1	-12.9	81.4	29.3	39.2	48.1	55.6	65.9	73.2	83.6
61		1	none	1	-22.1	86.2	33.8	45.4	55.8	64.6	77.0	85.8	98.5
62		1	none	1	2.8	78.2	27.2	36.5	44.4	50.9	59.7	65.7	74.2
63		1	none	1	3.8	85.7	32.3	43.0	52.4	60.1	70.9	78.4	89.2

64		1	none	1	4.8	84.5	32.3	43.0	52.3	60.1	70.8	78.4	89.2
65		4	none	1	35.0	79.6	31.5	42.5	52.0	59.9	70.7	78.3	89.1
66		1	2	2	9.3	86.7	30.8	40.6	49.3	56.4	66.1	73.0	83.0
67		1	2	2	2.6	94.2	34.2	45.7	56.2	64.9	76.9	85.5	97.8
68		1	2	2	-21.0	97.5	38.8	52.2	64.2	74.3	88.3	98.3	112.7
69		2	none	1	47.7	76.5	26.9	36.2	44.6	51.6	61.3	68.2	78.1
70		2(C _{2v}) 1(C _s)	none	1	14.0	80.8	30.9	41.9	52.0	60.4	72.2	80.7	93.0

71		2	none	1	5.2	85.9	35.4	48.1	59.6	69.4	83.3	93.2	107.8
72		2	none	1	97.8	74.9	25.7	34.1	41.3	47.2	55.2	60.8	68.8
73		1	none	1	38.2	79.9	29.4	39.6	48.5	56.0	66.1	73.3	83.6
74		1	none	1	29.7	85.3	33.8	45.6	56.1	64.8	77.1	85.8	98.5
75		2	none	1	32.8	86.7	34.0	45.6	56.0	64.7	77.0	85.8	98.5
76		1	2	1	55.3	89.1	30.6	39.7	47.9	54.7	63.9	70.3	79.2

77		1	2	1	33.3	92.6	34.7	45.6	55.4	63.6	74.9	82.9	94.2
78		1	2	1	7.6	96.4	38.7	51.4	62.8	72.5	85.9	95.5	109.2
79		1	none	1	88.8	78.9	27.1	36.0	43.8	50.1	58.8	64.9	73.7
80		1	none	1	49.7	86.1	31.1	41.7	51.1	58.9	69.8	77.5	88.5
81		1	none	1	58.2	83.5	31.7	42.1	51.4	59.2	69.9	77.6	88.6
82		1	none	1	39.2	88.3	35.5	47.7	58.7	67.9	80.8	90.0	103.4

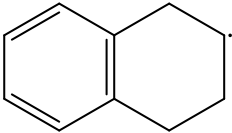
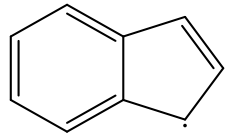
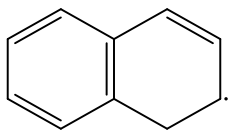
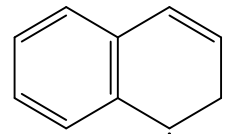
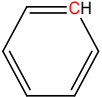
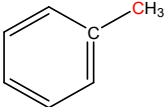
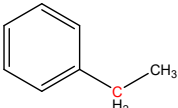
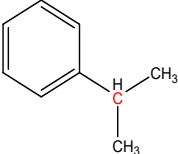
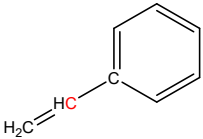
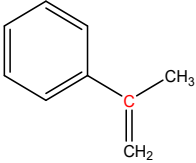
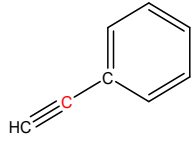
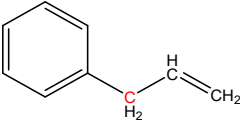
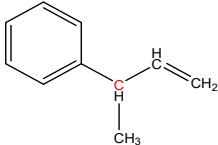
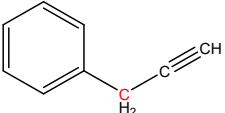
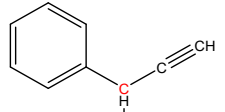
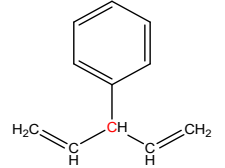
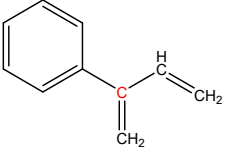
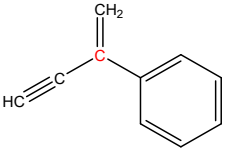
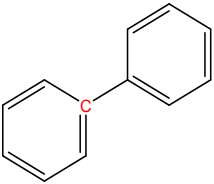
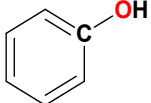
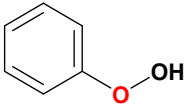
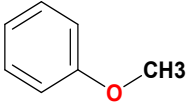
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84		1	none	1	66.1	79.2	29.0	38.9	47.3	54.2	63.5	69.9	79.1
85		1	none	1	57.7	87.3	33.7	45.1	55.0	63.2	74.6	82.6	94.1
86		1	none	1	62.3	86.6	33.8	45.2	55.1	63.2	74.6	82.6	94.1

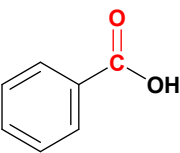
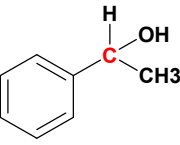
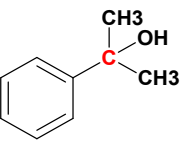
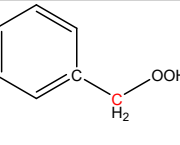
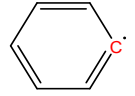
Table S 7 The comparison of GAVs against THERM data. The table provides the GAVs calculated in this work and the deviations from THERM. Relevant aromatic species are also provided.

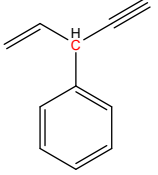
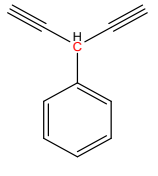
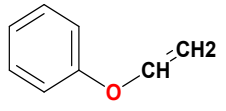
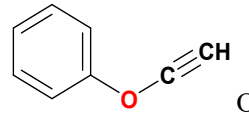
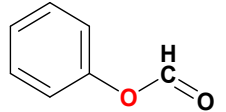
Group	$\Delta H_f(298.15\text{K})$ [kcal/mol]	$S(298.15\text{K})$ [cal/mol/K]	Cp [cal/mol/K]						
			300 K	400 K	500 K	600 K	800 K	1000 K	1500 K
 CB/H	3.36	11.53	3.27	4.42	5.46	6.33	7.51	8.35	9.58
	3.30	11.53	3.24	4.44	5.46	6.30	7.54	8.41	9.73
 C/CB/H3	-10.15	30.13	5.86	7.57	9.35	10.96	12.86	14.48	16.85
	-10.01	30.29	6.22	7.74	9.24	10.62	12.84	14.59	17.35
 C/CB/C/H2	-5.11	9.56	5.24	6.81	8.41	9.78	11.09	12.21	13.71
	-4.86	9.34	5.84	7.61	8.98	10.01	11.49	12.54	13.76
 C/C2/CB/H	-1.70	-11.73	5.04	6.60	7.94	8.93	9.56	10.07	10.63
	-0.98	-12.15	4.88	6.66	7.90	8.75	9.73	10.25	10.68
 CD/CB/H	7.27	6.27	3.20	4.77	6.21	7.39	8.31	9.03	9.95

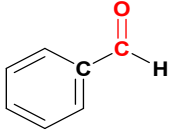
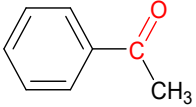
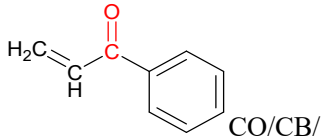
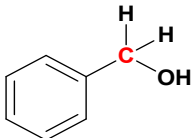
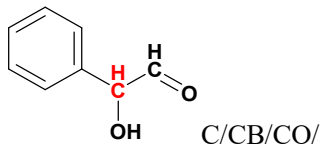
	6.78	6.38	4.46	5.79	6.75	7.42	8.35	9.11	10.09
 CD/C/CB	10.07	-17.33	4.28	6.02	7.41	8.44	9.13	9.65	10.19
	8.64	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
 CT/CB	26.93	5.12	2.42	3.31	4.07	4.63	4.89	5.13	5.41
	24.67	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
 C/CB/CD/H2	-5.08	12.64	3.88	5.07	6.30	7.41	8.31	9.15	10.21
	-4.29	2.00	4.51	6.76	8.61	10.01	11.97	13.40	15.47
 C/C/CB/CD/H	-1.39	-9.16	3.97	4.77	5.67	6.48	6.80	7.09	7.21
	-1.56	-11.77	4.50	6.57	8.07	8.89	9.88	10.39	10.79

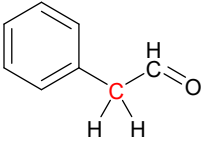
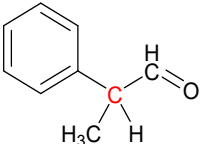
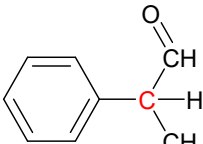
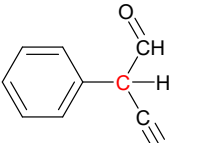
 <chem>C#CCc1ccccc1</chem> C/CB/CT/H2	-3.57	9.43	4.66	6.49	8.20	9.63	11.02	12.22	12.81
	-4.29	9.84	4.28	6.43	8.16	9.50	11.36	12.74	13.70
 <chem>C#CCc1ccccc1</chem> C/C/CB/CT/H	-0.37	-12.16	5.22	6.88	8.19	9.16	9.76	10.27	9.81
	-1.55	-11.65	4.33	6.27	7.58	8.48	9.52	10.10	10.63
 <chem>C=CC(=C)c1ccccc1</chem> C/CB/CD2/H	-0.80	-2.38	4.12	4.20	4.32	4.53	4.18	4.08	3.70
	-1.39	-11.39	4.12	6.51	8.24	9.00	10.03	10.53	10.89
 <chem>C=CC=Cc1ccccc1</chem> CD/CB/CD	9.41	-14.09	3.86	4.63	5.36	5.99	6.17	6.43	6.61
	7.18	-16.50	4.70	6.13	6.87	7.10	7.20	7.16	7.06
 <chem>C=CC=Cc1ccccc1</chem>	8.81	-14.22	2.69	3.77	5.42	5.18	5.64	6.07	6.37

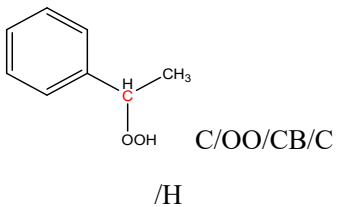
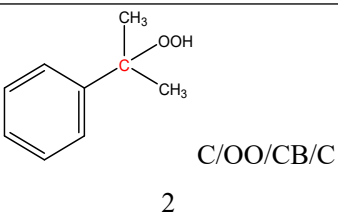
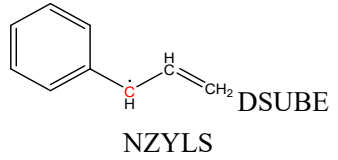
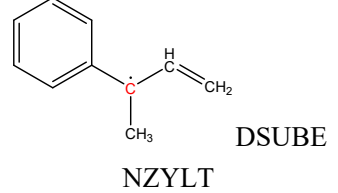
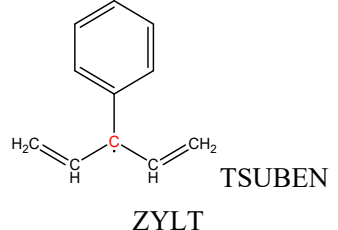
CD/CB/CT	6.70	-17.04	2.22	3.14	4.54	4.11	5.06	5.79	6.71
 CB/CB	4.57	-9.21	3.47	4.04	4.69	5.23	5.53	5.75	5.70
	4.96	-8.64	3.33	4.22	4.89	5.27	5.76	5.95	6.05
 O/CB/H	-37.54	29.12	4.70	4.69	4.97	5.43	5.83	6.34	6.70
	-37.90	29.10	4.30	4.50	4.82	5.23	6.02	6.61	7.44
 O/CB/O	0.58	11.04	2.60	2.22	2.33	2.62	3.03	3.39	3.26
	-1.98	10.70	2.85	2.92	3.02	3.09	3.48	3.66	3.23
 O/CB/C	-22.73	8.19	3.13	2.80	2.88	3.21	3.29	3.54	3.30
	-22.60	9.70	3.40	3.70	3.70	3.80	4.40	4.60	□

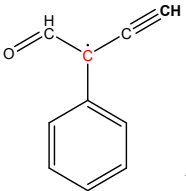
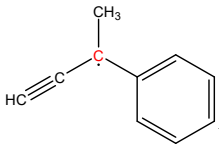
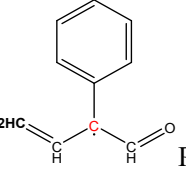
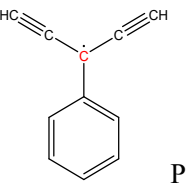
 CO/CB/O	-36.39	13.72	6.92	7.61	8.45	9.43	10.50	11.22	□
	-36.60	14.78	5.97	6.70	7.40	8.02	8.87	9.36	□
 C/CB/C/H/O	-6.45	-14.47	7.29	8.80	9.76	10.27	10.16	10.15	9.35
	-6.00	-11.10	4.47	6.82	8.45	9.17	10.24	10.80	11.02
 C/CB/C2/O	-5.34	-36.11	5.78	7.72	8.92	9.44	8.76	8.22	6.39
	-6.60	-32.56	4.63	6.79	7.95	8.40	8.80	8.44	□
 C/OO/CB/H2	-6.96	7.06	4.79	5.63	7.30	8.20	9.55	10.60	□
	-6.41	4.68	4.31	5.66	7.64	8.62	10.38	11.40	□
 PH	113.47	1.09	-0.50	-1.08	-1.67	-2.19	-2.94	-3.53	-4.48
	113.00	1.48	-0.41	-1.18	-1.93	-2.69	-3.75	-4.48	-5.24

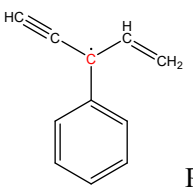
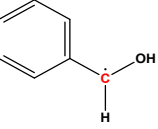
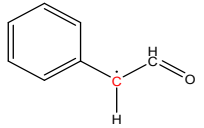
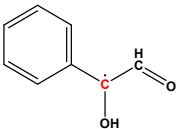
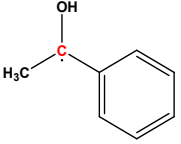
 <p>C/CB/CD/CT/H</p>	0.46	-9.05	3.35	4.67	5.74	6.56	6.76	7.07	6.23
 <p>C/CB/CT2/H</p>	5.40	-11.37	3.48	5.54	7.16	8.38	9.22	9.95	8.75
 <p>O/CB/CD</p>	-25.73	59.61	7.36	8.36	9.97	11.84	14.40	16.62	19.54
 <p>O/CB/C T</p>	-17.92	10.00	2.43	2.19	2.36	2.26	2.84	3.32	
 <p>O/CB/CO</p>	-36.78	7.06	2.50	2.89	3.37	3.79	3.82	3.85	3.18

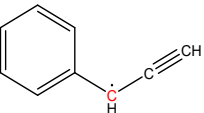
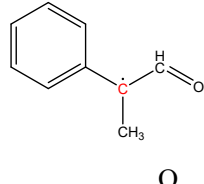
 <p>CO/CB/H</p>	-32.64	33.20	7.23	8.30	9.40	10.49	11.84	12.66	
 <p>CO/CB/C</p>	-33.35	13.02	6.68	7.49	8.28	9.24	10.00	10.35	
 <p>CO/CB/ CD</p>	-32.18	11.20	1.83	2.42	3.02	3.62	3.94	4.03	
 <p>C/CB/O/H2</p>	-6.63	7.69	6.19	7.94	9.40	10.47	11.21	11.96	12.25
 <p>C/CB/CO/</p>	-6.46	-19.09	6.31	9.54	11.93	13.21	13.17	12.66	24.70

O/H									
 <p>C/CB/CO/ H₂</p>	-4.82	9.70	5.02	6.76	8.35	9.50	10.73	11.71	27.30
 <p>C/CB/CO/ H/C</p>	-1.85	-13.61	7.23	8.49	9.17	9.43	9.64	9.81	24.33
 <p>C/CB/CO/ CD/H</p>	-0.52	-10.83	6.25	6.98	7.39	7.49	7.13	6.97	20.91
 <p>C/CB/CO/C T/H</p>	1.28	-13.47	6.68	8.29	9.33	9.83	9.99	10.16	23.58

 <p>C/OO/CB/C /H</p>	-6.76	-15.70	6.09	6.59	7.84	8.28	8.72	9.00	
 <p>C/OO/CB/C 2</p>	-5.51	-38.46	6.73	7.64	8.69	8.64	8.10	7.54	
 <p>DSUBE NZYLS</p>	78.81	-4.29	0.23	0.65	0.78	0.67	-0.04	-0.80	-2.44
 <p>DSUBE NZYLT</p>	79.31	-1.20	-1.19	-0.90	-1.00	-1.25	-1.77	-2.32	-3.48
 <p>TSUBEN ZYLT</p>	73.36	-6.85	-0.34	0.36	0.73	0.74	-0.08	-0.92	-2.69

 <p>PHCJ(C≡C) CO</p>	75.31	-1.57	-2.01	-1.81	-1.63	-1.54	-1.69	-2.00	-2.97
 <p>PHCJ(C) C≡C</p>	78.94	0.26	-0.70	-1.22	-1.66	-2.01	-2.46	-2.87	-3.76
 <p>PHCJ(C=C)C O</p>	78.17	-1.95	-1.58	-1.45	-1.30	-1.21	-1.28	-1.60	-2.69
 <p>PHCJ(C≡C)C ≡C</p>	70.67	-1.26	0.79	0.32	-0.28	-0.86	-1.61	-2.26	-3.43

 <p>PHCJ(C=C)C ≡C</p>	72.22	-2.61	-0.17	0.04	-0.08	-0.35	-1.00	-1.70	-3.15
 <p>PHCJO</p>	83.62	-2.20	0.48	0.41	0.11	-0.30	-1.20	-1.92	-3.16
 <p>PHCJCO</p>	83.58	-4.74	0.96	0.84	0.44	-0.03	-0.78	-1.42	-2.58
 <p>PHCJ(O)CO</p>	72.09	-1.42	-1.90	-3.01	-3.90	-4.36	-3.92	-3.11	-1.76
 <p>PHCJ(C)O</p>	83.91	1.55	-2.67	-2.62	-2.51	-2.48	-2.79	-3.05	-3.75

 $\text{PhC}\overset{\cdot}{\text{C}}\equiv\text{C}$	79.93	-1.79	0.50	0.30	-0.16	-0.67	-1.46	-2.14	-3.33
 $\text{PhC}(\overset{\cdot}{\text{C}})\text{C}$ O	82.70	-0.14	-2.67	-2.70	-2.51	-3.08	-2.45	-2.67	-3.39