Electronic Supplementary Material (ESI) for New Journal of Chemistry.

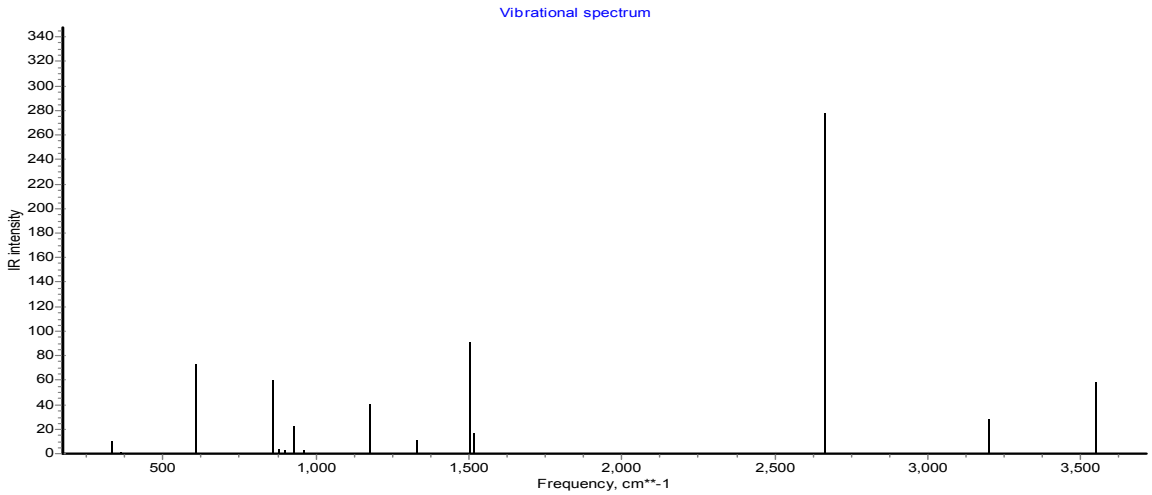
Introducing “carborazine” as a novel heterocyclic aromatic species

Ambrish Kumar Srivastava and Neeraj Misra*

This is supplementary material submitted to New Journal of Chemistry

Vibrational spectrum of carborazine (Frequency in cm^{-1}, Intensity in a.u.)

Frequency	Intensity
333.1137	10.7137
365.1717	0.8234
608.3296	73.8774
860.4568	60.3777
879.7261	3.8198
902.4997	2.4389
930.374	22.4256
964.5922	3.2394
1178.2877	40.4436
1330.2551	11.7221
1503.8589	91.0484
1517.6084	16.6591
2662.1762	278.2399
3202.5922	28.3156
3552.512	58.2137



Cartesian co-ordinates

	Atomic Number	x	y	z
A.	Benzene (Figure 1)			
	6	0.000000000	1.407958000	0.000000000
	6	1.219328000	0.703979000	0.000000000
	6	1.219328000	-0.703979000	0.000000000
	6	0.000000000	-1.407958000	0.000000000
	6	-1.219328000	-0.703979000	0.000000000
	6	-1.219328000	0.703979000	0.000000000
	1	0.000000000	2.502167000	0.000000000
	1	2.166940000	1.251084000	0.000000000
	1	2.166940000	-1.251084000	0.000000000
	1	0.000000000	-2.502167000	0.000000000
	1	-2.166940000	-1.251084000	0.000000000
	1	-2.166940000	1.251084000	0.000000000
B.	Borazine (Figure 1)			
	1	0.000000000	-2.665521000	0.000000000
	1	2.105816000	-1.215794000	0.000000000
	1	2.308409000	1.332761000	0.000000000
	1	0.000000000	2.431587000	0.000000000
	1	-2.308409000	1.332761000	0.000000000
	1	-2.105816000	-1.215794000	0.000000000
	5	-1.267187000	0.731611000	0.000000000
	5	1.267187000	0.731611000	0.000000000
	5	0.000000000	-1.463222000	0.000000000
	7	0.000000000	1.417628000	0.000000000
	7	-1.227702000	-0.708814000	0.000000000
	7	1.227702000	-0.708814000	0.000000000
C.	Carborazine (Figure 1)			
	1	1.167539000	-2.109956000	0.000000000
	1	-1.103375000	-2.287152000	0.000000000
	1	-2.684973000	0.094173000	0.000000000
	1	-1.167539000	2.109956000	0.000000000
	1	1.103375000	2.287152000	0.000000000
	1	2.684973000	-0.094173000	0.000000000
	5	-1.487741000	0.000370000	0.000000000
	7	-0.685937000	1.210845000	0.000000000
	6	-0.685937000	-1.274769000	0.000000000
	6	0.685937000	1.274769000	0.000000000
	7	0.685937000	-1.210845000	0.000000000
	5	1.487741000	-0.000370000	0.000000000
D.	Carborazine isomer (Figure 2)			
	1	-2.118375000	-1.249158000	0.000000000
	1	-2.288176000	1.323056000	0.000000000
	1	0.044592000	2.366017000	0.000000000
	1	2.103403000	1.329292000	0.000000000
	1	2.294659000	-1.121848000	0.000000000
	1	-0.057956000	-2.715782000	0.000000000
	7	-1.233692000	-0.750229000	0.000000000
	5	-0.005669000	-1.512037000	0.000000000
	5	-1.271891000	0.683639000	0.000000000
	7	0.000000000	1.353539000	0.000000000
	6	1.216333000	0.686007000	0.000000000
	6	1.291250000	-0.688133000	0.000000000
E.	Phenol analog of carborazine (Figure 4, isomer 1)			
	1	-1.918310000	-1.891615000	-0.000120000
	1	-3.001705000	0.116270000	-0.000200000
	1	-1.439788000	2.523125000	-0.000126000
	1	1.037088000	1.911597000	0.000143000
	1	0.550076000	-2.473362000	0.000020000
	5	-1.058406000	1.385239000	0.000033000

7	0.375627000	1.131753000	0.000125000
6	-1.908043000	0.144293000	-0.000104000
6	0.969714000	-0.093608000	0.000147000
7	-1.291583000	-1.086687000	0.000013000
5	0.130870000	-1.346388000	0.000078000
8	2.345118000	-0.010602000	-0.000263000
1	2.691033000	-0.915020000	0.000608000

F. Phenol analog of carborazine (Figure 4, isomer 2)

1	2.871374000	0.022358000	0.000179000
1	1.921800000	-2.058049000	0.000033000
1	-0.937724000	-2.281951000	-0.000079000
1	1.813798000	2.322264000	0.000166000
5	-0.251309000	-1.294468000	-0.000130000
7	-0.916332000	-0.003821000	-0.000163000
6	1.242907000	-1.199189000	-0.000006000
6	-0.336182000	1.224939000	-0.000110000
7	1.852107000	0.032228000	0.000073000
5	1.168557000	1.310953000	0.000052000
1	-1.049232000	2.054173000	-0.000011000
8	-2.326641000	0.049342000	0.000049000
1	-2.583910000	-0.889310000	0.001043000

G. Phenol analog of carborazine (Figure 4, isomer 3)

1	-0.829866000	2.044018000	0.000231000
1	1.442236000	2.360328000	0.000043000
1	3.161452000	0.072689000	0.000174000
5	1.961014000	0.101347000	0.000125000
7	1.228991000	-1.153869000	-0.000010000
6	1.087197000	1.324692000	-0.000147000
6	-0.136732000	-1.310362000	-0.000091000
7	-0.280769000	1.182823000	0.000006000
5	-1.008788000	-0.072633000	-0.000041000
1	-0.488302000	-2.348415000	0.000100000
8	-2.412891000	0.035802000	0.000057000
1	-2.847784000	-0.824877000	-0.000047000
1	1.763920000	-2.022387000	0.000083000

H. Aniline analog of carborazine (Figure 4, isomer 1)

1	-1.944126000	-1.885694000	0.015503000
1	-3.025507000	0.127110000	0.017760000
1	-1.448636000	2.525682000	0.003330000
1	0.994007000	1.925570000	-0.059929000
1	0.508755000	-2.474720000	0.008135000
5	-1.073113000	1.384697000	0.002861000
7	0.358223000	1.126406000	-0.014598000
6	-1.931552000	0.149697000	0.010762000
6	0.969881000	-0.102352000	-0.006401000
7	-1.317527000	-1.080850000	0.004294000
5	0.106504000	-1.340885000	-0.001692000
7	2.374512000	-0.092379000	-0.077049000
1	2.832481000	0.614361000	0.497121000
1	2.779640000	-1.007685000	0.097547000

I. Aniline analog of carborazine (Figure 4, isomer 2)

1	0.782289000	2.062432000	-0.009477000
1	-1.468511000	2.358233000	0.000495000
1	-3.187383000	0.076077000	0.003118000
1	-1.784851000	-2.021763000	0.002637000
5	-1.986446000	0.100224000	0.002106000
7	-1.253529000	-1.151123000	0.001562000
6	-1.110957000	1.323029000	0.001185000
6	0.113621000	-1.304332000	0.002068000
7	0.258296000	1.186641000	-0.000974000
5	0.998950000	-0.072868000	0.000130000
1	0.464346000	-2.342646000	0.002932000

7	2.445725000	-0.066679000	-0.044221000
1	2.993402000	0.756630000	0.172454000
1	2.968757000	-0.919800000	0.102566000

J. Aniline analog of carborazine (Figure 4, isomer 3)

1	-2.895138000	0.008998000	0.000307000
1	-1.935637000	-2.064322000	-0.000137000
1	0.902881000	-2.287113000	-0.000437000
5	0.240593000	-1.284639000	-0.000268000
7	0.922674000	0.000886000	-0.000197000
6	-1.260251000	-1.202083000	-0.000115000
6	0.306924000	1.223938000	-0.000018000
7	-1.875405000	0.024062000	0.000188000
5	-1.197161000	1.307310000	0.000285000
1	1.007788000	2.063440000	-0.000226000
1	-1.851493000	2.313522000	0.000491000
7	2.370796000	0.070872000	-0.000354000
1	2.673960000	-0.471942000	0.813663000
1	2.673987000	-0.477804000	-0.810408000

K. Naphthalene analog of carborazine (Figure 5, structure 1)

6	0.000000000	1.326304000	-1.425534000
6	0.000000000	1.211130000	1.460256000
1	0.000000000	-1.432442000	-2.517423000
1	0.000000000	3.345356000	-1.246378000
1	0.000000000	1.432442000	-2.517423000
6	0.000000000	-1.326304000	-1.425534000
6	0.000000000	-1.211130000	1.460256000
1	0.000000000	1.104066000	2.552108000
1	0.000000000	3.606991000	1.282035000
1	0.000000000	-1.104066000	2.552108000
1	0.000000000	-3.606991000	1.282035000
1	0.000000000	-3.345356000	-1.246378000
5	0.000000000	2.528338000	0.752918000
5	0.000000000	0.000000000	-0.706475000
5	0.000000000	-2.528338000	0.752918000
7	0.000000000	0.000000000	0.783767000
7	0.000000000	2.476196000	-0.713286000
7	0.000000000	-2.476196000	-0.713286000

L. Naphthalene analog of carborazine (Figure 5, structure 2)

1	0.000000000	-1.424045000	-2.648346000
1	0.000000000	3.444111000	-1.128937000
1	0.000000000	1.424045000	-2.648346000
1	0.000000000	1.222852000	2.671784000
1	0.000000000	3.544461000	1.148727000
1	0.000000000	-1.222852000	2.671784000
1	0.000000000	-3.544461000	1.148727000
1	0.000000000	-3.444111000	-1.128937000
7	0.000000000	0.000000000	0.706025000
7	0.000000000	2.540558000	-0.656521000
7	0.000000000	-2.540558000	-0.656521000
6	0.000000000	0.000000000	-0.696711000
6	0.000000000	-2.554084000	0.681447000
6	0.000000000	2.554084000	0.681447000
5	0.000000000	1.300773000	-1.453653000
5	0.000000000	1.255589000	1.475037000
5	0.000000000	-1.300773000	-1.453653000
5	0.000000000	-1.255589000	1.475037000

M. Naphthalene analog of carborazine (Figure 5, structure 3)

1	0.000000000	-1.135162000	-2.440499000
1	0.000000000	3.474712000	-1.459046000
1	0.000000000	1.135162000	-2.440499000
1	0.000000000	1.340693000	2.431161000
1	0.000000000	3.373797000	1.379694000

1	0.000000000	-1.340693000	2.431161000
1	0.000000000	-3.373797000	1.379694000
1	0.000000000	-3.474712000	-1.459046000
6	0.000000000	0.000000000	-0.787811000
6	0.000000000	-2.491876000	0.736574000
6	0.000000000	2.491876000	0.736574000
5	0.000000000	0.000000000	0.778226000
5	0.000000000	2.519969000	-0.731670000
5	0.000000000	-2.519969000	-0.731670000
7	0.000000000	1.280104000	1.413993000
7	0.000000000	1.168939000	-1.418773000
7	0.000000000	-1.168939000	-1.418773000
7	0.000000000	-1.280104000	1.413993000