

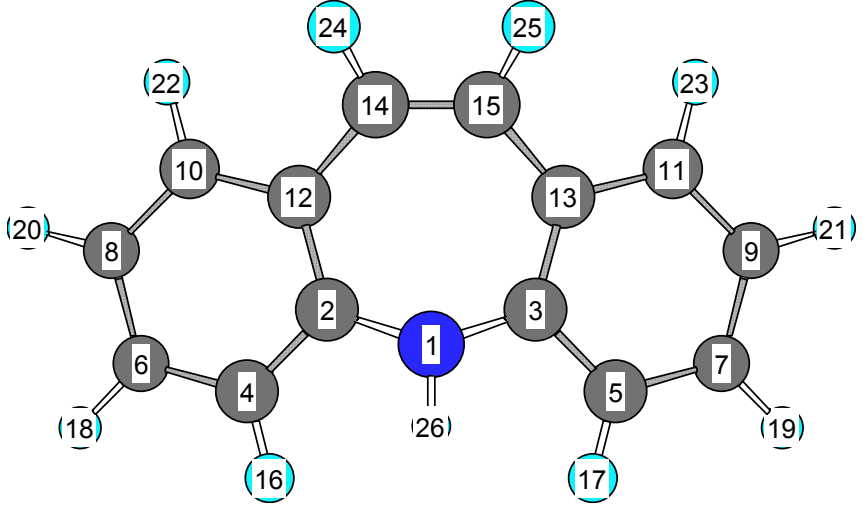
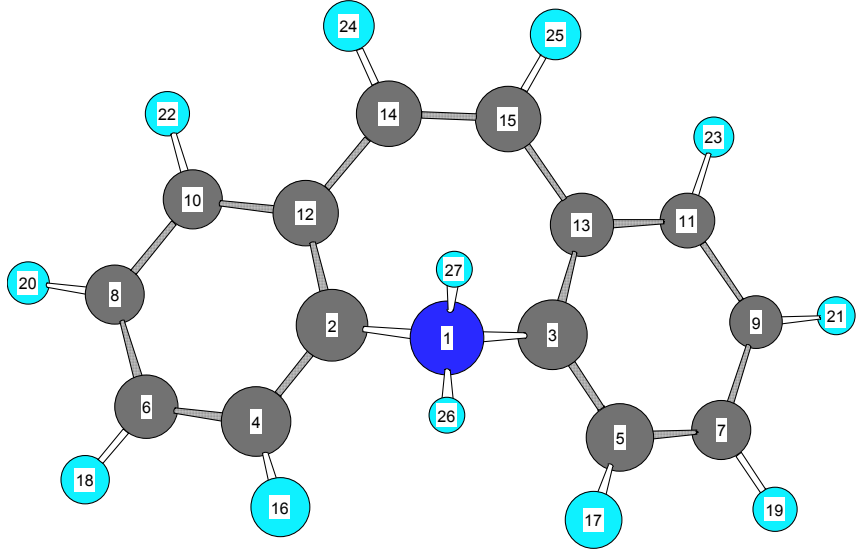
Supplementary Information

Org. Biomol. Chem., 2004, DOI: 10.1039/b314742h.

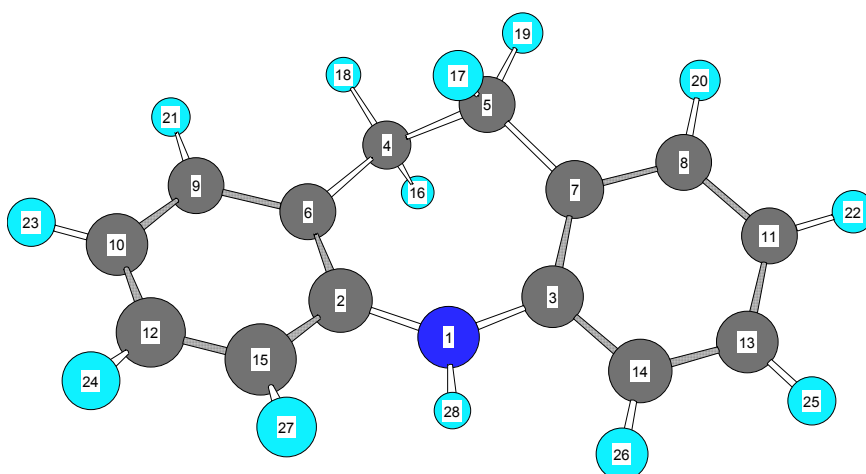
Homoheteroaromaticity: the case study of azepine and dibenzazepine

Christophe Dardonville,^{*} María Luisa Jimeno, Ibon Alkorta and José Elguero

Absolute chemical shieldings calculated at the B3LYP/6-311++G**//B3LYP/6-311++G** computational level.

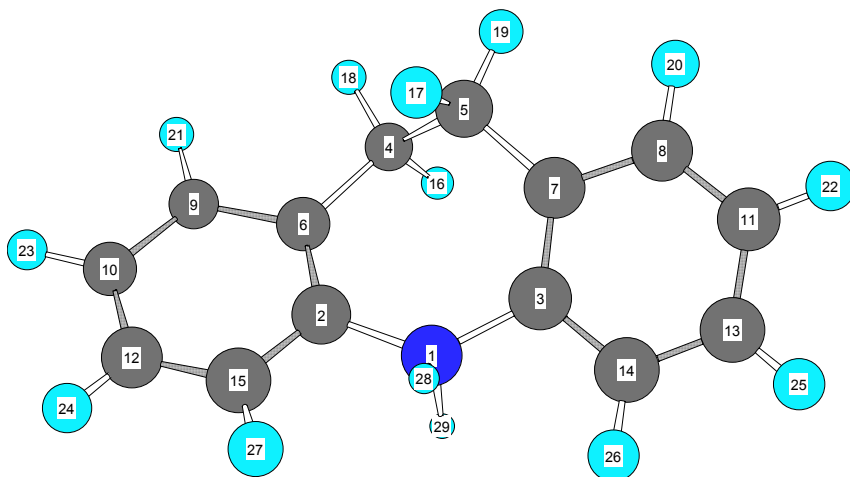
<p>1b</p> 	<table border="0"> <tbody> <tr><td>1 N</td><td>139.9911</td></tr> <tr><td>2 C</td><td>25.5706</td></tr> <tr><td>3 C</td><td>25.5706</td></tr> <tr><td>4 C</td><td>60.6005</td></tr> <tr><td>5 C</td><td>60.6005</td></tr> <tr><td>6 C</td><td>48.4259</td></tr> <tr><td>7 C</td><td>48.4259</td></tr> <tr><td>8 C</td><td>55.6413</td></tr> <tr><td>9 C</td><td>55.6413</td></tr> <tr><td>10 C</td><td>47.5294</td></tr> <tr><td>11 C</td><td>47.5294</td></tr> <tr><td>12 C</td><td>44.8308</td></tr> <tr><td>13 C</td><td>44.8308</td></tr> <tr><td>14 C</td><td>43.4719</td></tr> <tr><td>15 C</td><td>43.4719</td></tr> <tr><td>16 H</td><td>25.5574</td></tr> <tr><td>17 H</td><td>25.5574</td></tr> <tr><td>18 H</td><td>24.8187</td></tr> <tr><td>19 H</td><td>24.8187</td></tr> <tr><td>20 H</td><td>25.1462</td></tr> <tr><td>21 H</td><td>25.1462</td></tr> <tr><td>22 H</td><td>25.1441</td></tr> <tr><td>23 H</td><td>25.1441</td></tr> <tr><td>24 H</td><td>25.6739</td></tr> <tr><td>25 H</td><td>25.6739</td></tr> <tr><td>26 H</td><td>27.5952</td></tr> </tbody> </table>	1 N	139.9911	2 C	25.5706	3 C	25.5706	4 C	60.6005	5 C	60.6005	6 C	48.4259	7 C	48.4259	8 C	55.6413	9 C	55.6413	10 C	47.5294	11 C	47.5294	12 C	44.8308	13 C	44.8308	14 C	43.4719	15 C	43.4719	16 H	25.5574	17 H	25.5574	18 H	24.8187	19 H	24.8187	20 H	25.1462	21 H	25.1462	22 H	25.1441	23 H	25.1441	24 H	25.6739	25 H	25.6739	26 H	27.5952		
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4b



1 N	130.7880
2 C	34.8775
3 C	34.8775
4 C	142.0752
5 C	142.0752
6 C	49.0496
7 C	49.0496
8 C	46.7218
9 C	46.7218
10 C	60.0214
11 C	60.0214
12 C	50.8476
13 C	50.8476
14 C	62.0090
15 C	62.0090
16 H	28.8818
17 H	28.8818
18 H	28.9436
19 H	28.9436
20 H	24.7939
21 H	24.7939
22 H	25.1661
23 H	25.1661
24 H	24.7550
25 H	24.7550
26 H	25.2478
27 H	25.2478
28 H	26.1839

5b



1 N	160.8214
2 C	44.4769
3 C	41.8193
4 C	148.9060
5 C	150.6228
6 C	43.2850
7 C	42.6780
8 C	44.6917
9 C	41.4101
10 C	42.1744
11 C	41.3884
12 C	47.3789
13 C	46.4752
14 C	59.0792
15 C	57.6056
16 H	28.5725
17 H	28.5060
18 H	28.3664
19 H	28.5645
20 H	23.9507
21 H	24.1138
22 H	23.8049
23 H	23.8037
24 H	24.1356
25 H	24.0888
26 H	24.4143
27 H	24.7359
28 H	23.4908
29 H	25.7190