

Is Azulene's local aromaticity and relative stability driven by the Glidewell–Lloyd rule?

Rodrigo Báez-Grez¹ and Ricardo Pino Rios^{2,3*}

¹Facultad de Ciencias, Universidad Arturo Prat, Casilla 121, Iquique 1100000, Chile.

²Centro de Investigación Medicina de Altura – CEIMA, Universidad Arturo Prat. Casilla 121, Iquique 1100000, Chile. rpinoarios@unap.cl.

³Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat, Casilla 121, Iquique 1100000, Chile.

SUPPORTING INFORMATION

Figure S1. Scheme showing the formation of the local aromatic rings ($C_7H_7^+$ and $C_5H_5^-$) in azulene from the globally aromatic ring.

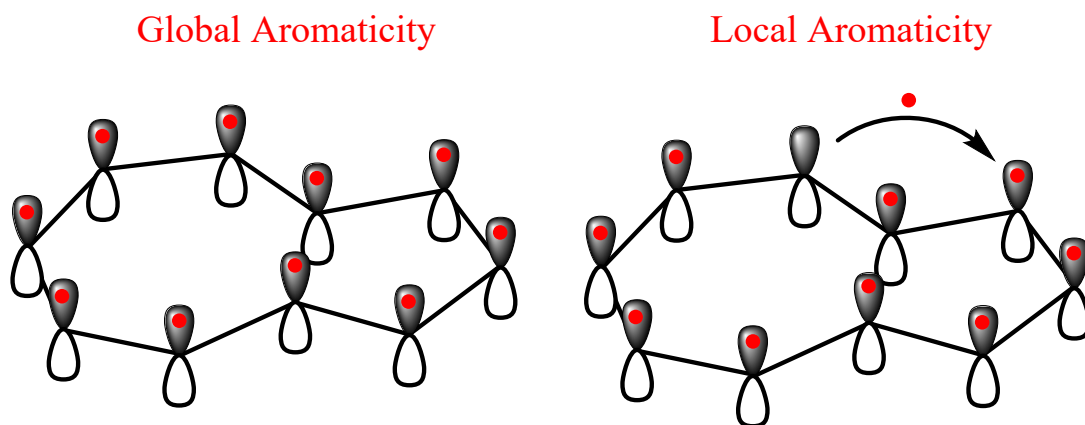
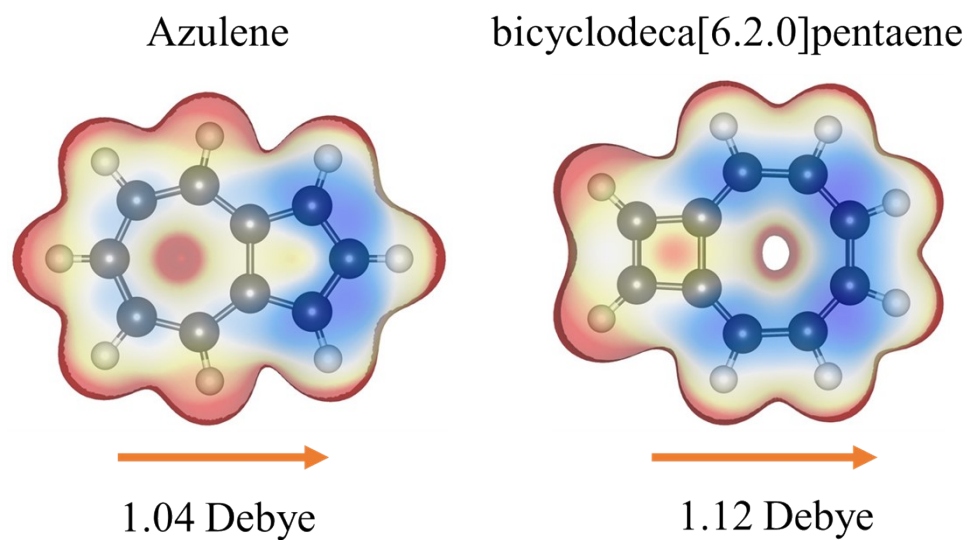


Figure S2. Electrostatic potential maps for Azulene and bicyclodeca[6.2.0]pentaene computed at the B3LYP/6-311G** level. Blue values are for negative charge and red values for positive charge. Orange arrows represent the direction of the dipole moment.



CARTESIAN COORDINATES

Azulene				
C	0.553077042	0.749293055	0.000000000	
C	0.553077042	-0.749293055	0.000000000	
C	-0.551544042	-1.592467113	0.000000000	
C	-1.907938136	-1.264084092	0.000000000	
C	-2.499007178	0.000000000	0.000000000	
C	-1.907938136	1.264084092	0.000000000	
C	-0.551544042	1.592467113	0.000000000	
H	-0.323558023	-2.656234190	0.000000000	
H	-2.595692185	-2.103929154	0.000000000	
H	-3.585810256	0.000000000	0.000000000	
H	-2.595692185	2.103929154	0.000000000	
H	-0.323558023	2.656234190	0.000000000	
C	1.899243135	1.148534080	0.000000000	
C	2.704517195	0.000000000	0.000000000	
C	1.899243135	-1.148534080	0.000000000	
H	2.245126164	2.172680158	0.000000000	
H	3.786938272	0.000000000	0.000000000	
H	2.245126164	-2.172680158	0.000000000	
Naphthalene				
C	1.400284335	1.243509781	0.000000000	
C	0.707411809	2.429398420	0.000000000	
C	-0.707411809	2.429398420	0.000000000	
C	-1.400284335	1.243509781	0.000000000	
C	-0.715625926	0.000000000	0.000000000	
C	0.715625926	0.000000000	0.000000000	
C	1.400284335	-1.243509781	0.000000000	
C	0.707411809	-2.429398420	0.000000000	
C	-0.707411809	-2.429398420	0.000000000	
C	-1.400284335	-1.243509781	0.000000000	
H	1.242846621	3.372195280	0.000000000	
H	-1.242846621	3.372195280	0.000000000	
H	-2.485454033	1.241908147	0.000000000	
H	-2.485454033	-1.241908147	0.000000000	
H	-1.242846621	-3.372195280	0.000000000	
H	1.242846621	-3.372195280	0.000000000	
H	2.485454033	-1.241908147	0.000000000	
H	2.485454033	1.241908147	0.000000000	
bicyclodeca[6.2.0]pentaene				
C	0.149695936	-1.778586192	0.000000000	
C	1.050819146	0.774618637	0.000000000	
C	-1.281461585	-1.726006061	0.000000000	
C	-1.281461585	1.726055867	0.000000000	
C	1.050868143	-0.774703030	0.000000000	
C	-2.209324392	0.717309032	0.000000000	
C	-2.209306103	-0.717243668	0.000000000	
C	0.149696286	1.778543424	0.000000000	
H	0.568988688	-2.782184323	0.000000000	
H	-1.730435507	-2.716114310	0.000000000	
H	-1.730406170	2.716176340	0.000000000	
H	-3.226914440	1.100779829	0.000000000	
H	-3.226888029	-1.100738886	0.000000000	
H	0.569049469	2.782115350	0.000000000	
C	2.478615005	0.697714191	0.000000000	
C	2.478663461	-0.697717229	0.000000000	
H	3.257839135	1.448211326	0.000000000	
H	3.257940975	-1.448155138	0.000000000	