JOC Additions and Corrections

Vol. 71, 2006

Giovanni F. Caramori, Kleber T. de Oliveira, Sérgio Emanuel Galembeck,* Patrick Bultinck, Mauricio G. Constantino. Aromaticity and Homoaromaticity in Methano[10]-annulenes.

Pages 83 and 84. In Tables 13 and 14, respectively, the symbol of the Laplacian of electron density was substituted by a line (-2). The correct tables are as follows:

TABLE 13. Properties of BCPs and RCPs (au)

			compounds				
critical points	properties	1	2	3			
BCPs (a) ^a							
C(1)-C(2)	$ ho_{ m b}$	0.278	0.300	0.299			
	$ abla^2 ho_{ m b}$	-0.700	-0.814	-0.819			
C(2)-C(3)	ϵ_{b}	0.370	0.406	0.403			
	$ ho_{ m b}$	0.310	0.292	0.304			
	$\nabla^2 ho_{ m b}$	-0.841	-0.765	-0.827			
	ϵ_{b}	0.425	0.398	0.415			
C(3)-C(4)	$ ho_{ m b}$	0.278	0.293	0.287			
	$\nabla^2 ho_{ m b}$	-0.701	-0.766	-0.748			
C(4)-C(5)	$\epsilon_{ m b}$	0.370	0.399	0.388			
	$ ho_{ m b}$		0.301	0.304			
	$\nabla^2 ho_{ m b}$		-0.816	-0.827			
	ϵ_{b}		0.407	0.415			
	В	CPs (b)					
C(4)-C(5)	$ ho_{ m b}$	0.324					
., .,	$\nabla^2 ho_{ m b}$	-0.939					
	ϵ_{b}	0.443					
C(5)-C(6)	$ ho_{ m b}$	0.280	0.307				
-(-) -(-)	$\nabla^2 \rho_{\rm b}$	-0.725	-0.861				
	ϵ_{b}	0.377	0.413				
C(6)-C(7)	$ ho_{ m b}$	0.303	0.297	0.299			
-(-)	$ abla^2 ho_{ m b}$	-0.812	-0.802	-0.819			
	ϵ_{b}	0.415	0.404	0.403			
C(7)-C(8)	$ ho_{ m b}$	0.267	0.289	0.304			
., .,	$\nabla^2 \rho_{\rm h}$	-0.649	-0.755	-0.827			
	ϵ_{b}	0.359	0.393	0.415			
C(8)-C(9)	$ ho_{ m b}$	0.303	0.289	0.287			
- (-)	$\nabla^2 \rho_{\rm b}$	-0.811	-0.752	-0.748			
	ϵ_{b}	0.415	0.392	0.388			
RCP (a)	$ ho_{ m b}$	0.050	0.024	0.013			
. ,	$\nabla^2 \rho_{\rm b}$	0.304	0.167	0.082			
	ϵ_{b}	0.058	0.016	0.003			
RCP (b)	$ ho_{ m b}$	0.014	0.014	0.013			
1101 (0)	$\nabla^2 \rho_{ m b}$	0.064	0.061	0.082			
	€ _b	0.010	0.008	0.003			
C(1)-C(11)	$ ho_{ m b}$	0.256	0.256	0.256			
- () -()	$\nabla^2 \rho_{\rm b}$	-0.618	-0.614	-0.612			
	ϵ_{b}	0.331	0.331	0.334			

^a The indexes (a) and (b) refer to the CPs from ring fragments (a) and (b).

TABLE 14. Bond Critical Points Parameters in au

compounds	CPs	$ ho_{ m b}$	$ abla^2 ho_{ m b}$	ϵ	G_{b}	V_{b}	H_{b}	$r_{\rm b}-r_{\rm r}$	$\rho_{ m r}- ho_{ m b}$	BL	BPL
1	ζ_1	0.016	0.064	6.960	0.014	-0.011	0.003	1.772	0.002	4.142	5.494
	BCP_{ring}	0.278	-0.700	0.149	0.091	-0.358	-0.266	1.872	0.228	2.734	2.736
2	ζ_2	0.014	0.055	3.186	0.012	-0.009	0.007	0.928	0.000	4.643	4.816
	BCP_{ring}	0.292	-0.765	0.398	0.105	-0.401	-0.296	2.241	0.268	2.669	2.670

JO070185T

10.1021/jo070185t Published on Web 02/09/2007