

The nature of resonance-assisted hydrogen bonds: a quantum chemical topology perspective

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Supporting Information

Table S1: Delocalization indices for atom pairs in the ring computed at the HF and MP2 levels.

System (a)					System (b)						
		HF		MP2				HF		MP2	
Pair	open	close	open	close	Pair	open	close	open	close		
C1 C2	1.02	1.11	0.92	1.00	C1 C2	0.95	0.95	0.84	0.84		
C2 C3	1.60	1.49	1.35	1.27	C2 C3	0.94	0.94	0.83	0.83		
C3 O4	0.87	0.92	0.84	0.90	C3 O4	0.78	0.80	0.76	0.77		
O4 H5	0.57	0.35	0.54	0.37	O4 H5	0.61	0.54	0.57	0.52		
C1 O6	1.27	1.17	1.21	1.13	C1 O6	1.29	1.28	1.23	1.22		

System (c)					System (d)						
		HF		MP2				HF		MP2	
Pair	open	close	open	close	Pair	open	close	open	close		
C1 C2	1.06	1.12	0.95	1.01	C1 C2	0.95	0.95	0.84	0.84		
C2 C3	1.56	1.45	1.32	1.25	C2 C3	0.95	0.94	0.83	0.83		
C3 N4	1.00	1.07	0.95	1.01	C3 N4	0.93	0.94	0.86	0.86		
N4 H5	0.78	0.61	0.69	0.58	N4 H5	0.87	0.82	0.76	0.72		
C1 O6	1.25	1.18	1.19	1.14	C1 O6	1.29	1.28	1.23	1.22		

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