Computer Modeling of Polyspin Organic Molecules Based on Bis-Triangulenes and Stable Radicals

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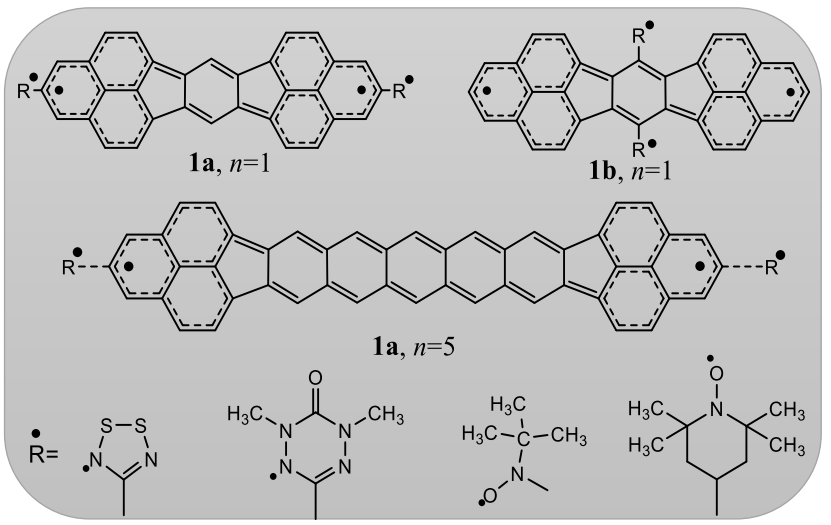
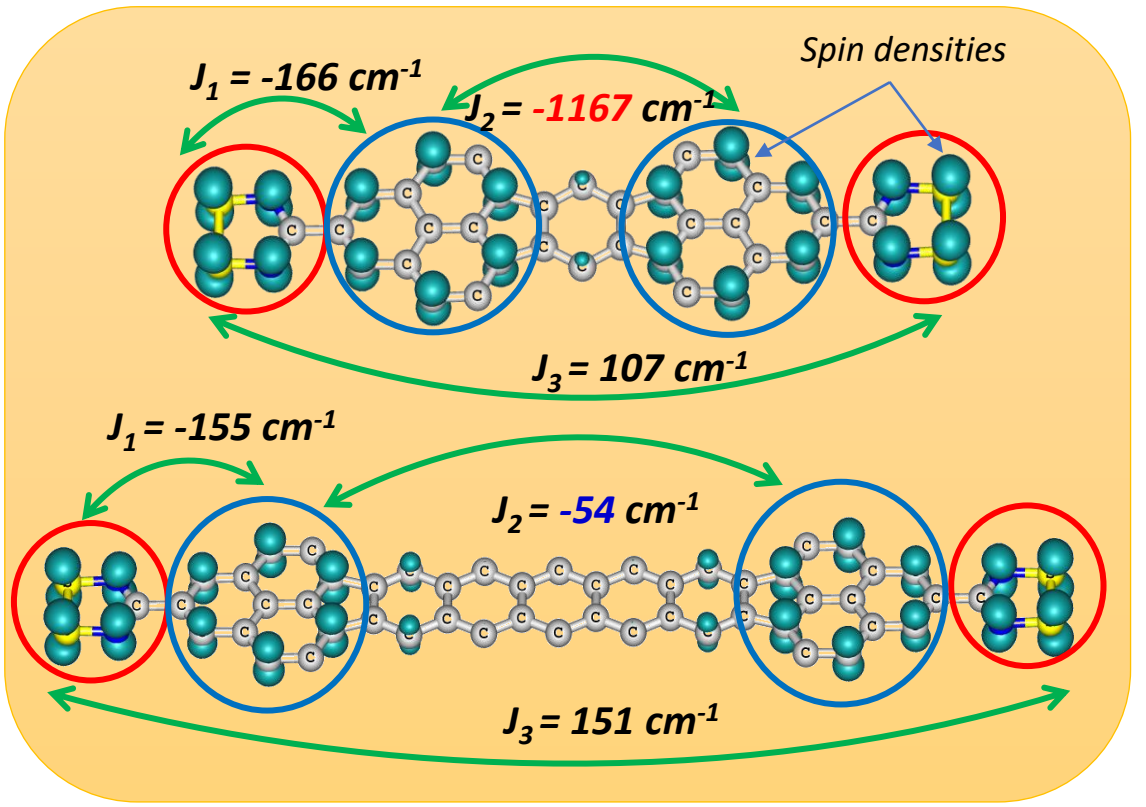
TETRARADICALS BASED ON BIS-PHENALENYL DERIVATIVES WITH STABLE RADICAL GROUPS



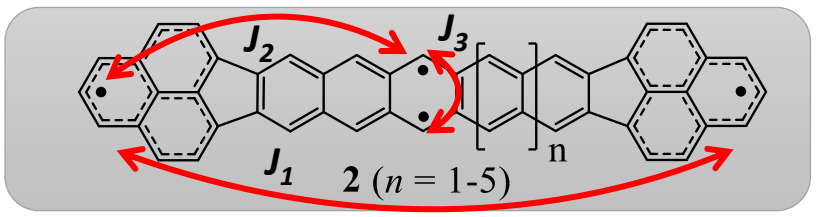


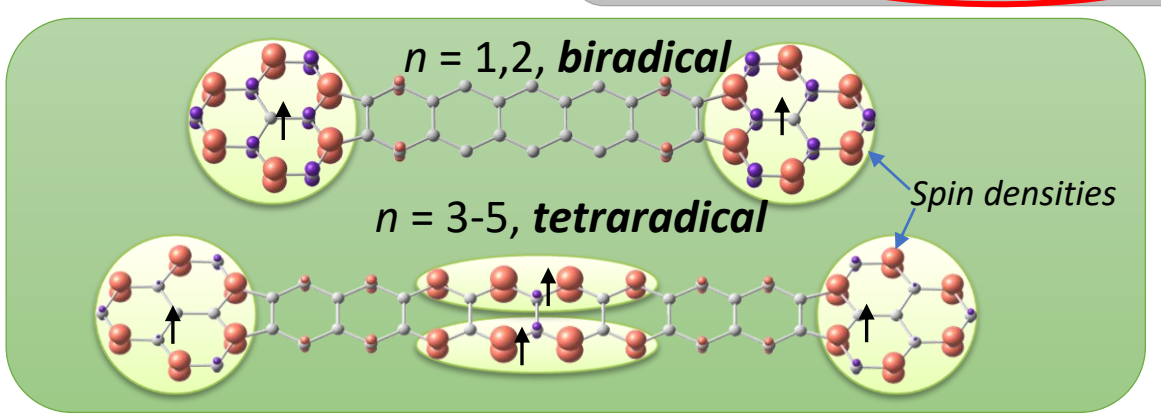
Compound	B3LYP/6-311++G(d,p)		
	y_0	y_1	N_U
1a (n = 1; R = TBN)	0.95	0.13	2.80
1a (n = 1; R = TEMPO)	1.00	0.12	2.84
1a (n = 1; R = VD)	0.97	0.14	2.88
1a (n = 3; R = DTDA)	0.95	0.42	3.34
1a (n = 3; R = TBN)	0.94	0.43	3.34
1a (n = 3; R = TEMPO)	0.99	0.38	3.37
1a (n = 3; R = VD)	0.95	0.41	3.34
1a (n = 5; R = DTDA)	0.95	0.62	3.62
1a (n = 5; R = TBN)	0.93	0.63	3.59
1a (n = 5; R = TEMPO)	1.00	0.62	3.65
1a (n = 5; R = VD)	0.96	0.61	3.60

(y_0) *biradicaloid indexes*
(y_1) *tetraradicaloid indexes*
(N_U) *effective number of unpaired electrons*

Increasing the size of the acene linker results in the appearance of exchange channels differing in nature, but similar in strength, which allows us to expect the existence of spin entanglement.

PURE HYDROCARBON TETRARADICALS BASED ON BIS-PHENALENYL DERIVATIVES





Compound	B3LYP/6-311++G(d,p)		
	y_0	y_1	N_U
2 (n = 1)	0.36	0.01	1.61
2 (n = 2)	0.43	0.02	1.89
2 (n = 3)	0.48	0.05	2.16
2 (n = 4)	0.52	0.10	2.50
2 (n = 5)	0.55	0.16	2.78

…Increasing the linker size leads to the formation of tetraradicaloids with two types of paramagnetic centers.
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