Supporting Information for

The Covalent Excited States of Polyenes $C_{2n}H_{2n+2}$
($n = 2-8$) and Polyenyl Radicals $C_{2n-1}H_{2n+1}$ ($n = 2-8$): An ab initio Valence Bond Study

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TABLE S1: C-C Bond Lengths of $C_{2n}H_{2n+2}$ Polyenes^{a,b}

$2n$	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8
4	1.3555	1.4676						
6	1.3578	1.4593	1.3651					
8	1.3588	1.4572	1.3683	1.4498				
10	1.3592	1.4564	1.3696	1.4472	1.3718			
12	1.3595	1.4558	1.3705	1.4458	1.3736	1.4439		
14	1.3596	1.4555	1.3708	1.4452	1.3745	1.4424	1.3754	
16	1.3597	1.4553	1.3711	1.4447	1.3750	1.4415	1.3765	1.4407

^a Optimized at the B3LYP/D95v level.^b Unique bond lengths are reported and are specified in order where the terminal bond is denoted as r_1 , etc.

TABLE S2: C-C Bond Lengths of $C_{2n-1}H_{2n+1}$ Polyenyl Radicals^{a,b}

$2n-1$	r_1	r_2	r_3	r_4	r_5	r_6	r_7
3	1.4008						
5	1.3796	1.4260					
7	1.3721	1.4366	1.4035				
9	1.3682	1.4422	1.3935	1.4154			
11	1.3661	1.4458	1.3877	1.4227	1.4050		
13	1.3647	1.4477	1.3841	1.4272	1.3985	1.4124	
15	1.3637	1.4491	1.3817	1.4305	1.3941	1.4176	1.4058

^a Optimized at the B3LYP/D95v level.^b Unique bond lengths are reported and are specified in order where the terminal bond is denoted as r_1 , etc.

Full reference for the Gaussian package

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision D.01; Gaussian, Inc.: Wallingford CT, 2004.