Supporting Information For the Article in Physical Chemistry Chemical Physics:

NMR Tensors in Planar Hydrocarbons of Increasing Size

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Table 1: Exponents of the completeness-optimized basis set co-b.

Element	s-type functions	p-type functions	d-type functions
H	775.923395	8.17053536	
	381.195457	4.44330808	
	162.434226	2.12132091	
	67.5426405	0.98850335	
	27.8580233	0.46067956	
	11.5613958	0.21993046	
	4.78717027	0.11960660	
	1.97894034		
	0.81614284		
	0.33844789		
	0.13992522		
C	7116275.08	775.9233956	8.17053536
	2926548.25	381.195457	4.44330808
	1020626.82	162.434226	2.12132091
	342377.699	67.5426405	0.98850335
	117115.463	27.8580233	0.46067956
	39299.1836	11.5613958	0.21993046
	13282.4240	4.78717027	0.11960660
	4501.74246	1.97894034	
	1517.23576	0.81614284	
	518.798211	0.33844789	
	173.682481	0.13992522	
	58.9418418		
	20.1640319		
	6.73534922		
	2.27415721		
	0.77216876		
	0.26119047		
	0.08842420		

Table 2: Exponents of the completeness-optimized basis set co-r.

Element	s-type functions	p-type functions	d-type functions
H	47.7400714	0.58854861	
	7.94070258	0.16796456	
	1.21658113		
	0.20235640		
C	6513146.63	650.102508	4.78898593
	2142103.89	215.899594	0.98855309
	613120.250	64.4251257	0.20405932
	171721.112	19.0878504	
	48138.7407	5.64954776	
	13515.7565	1.67204691	
	3792.83311	0.49487528	
	1067.44163	0.14650155	
	300.494366		
	84.1763651		
	23.7345565		
	6.66260853		
	1.85473217		
	0.52563999		
	0.14703558		

Table 3: Comparison of calculated NMR parameters for coronene, circumcoronene, and circumcircumcoronene using the full completeness-optimized co-r basis for all atoms and the locally dense basis sets (co-r* and co-r**). The PBE functional was used, and the couplings within the innermost carbon hexagon are considered. n denotes the number of basis functions. See text for details.

			Shielding		Spin-spin coupling					
System	Basis Set	n	σ	$\Delta\sigma$	^1J	Δ^1J	^2J	Δ^2J	^3J	Δ^3J
$C_{24}H_{12}$	co-r*	636	62.37	193.38	45.36	-3.24	0.42	-3.63	6.09	0.93
	co-r	1416	49.25	211.28	57.01	-1.64	0.18	-4.30	5.76	2.26
$C_{54}H_{18}$	co-r*	1086	54.13	206.47	58.20	-0.93	0.11	-4.79	6.24	3.24
	co-r**	1806	53.71	205.28	58.27	-0.97	0.10	-4.82	6.22	3.24
	co-r	3096	53.89	205.94	58.27	-1.00	0.10	-4.81	6.20	3.21
$C_{96}H_{24}$	co-r*	1704	53.90	209.61	58.60	-1.28	0.27	-4.53	5.91	2.75
	co-r**	2424	53.67	208.95	58.67	-1.32	0.26	-4.56	5.89	2.75

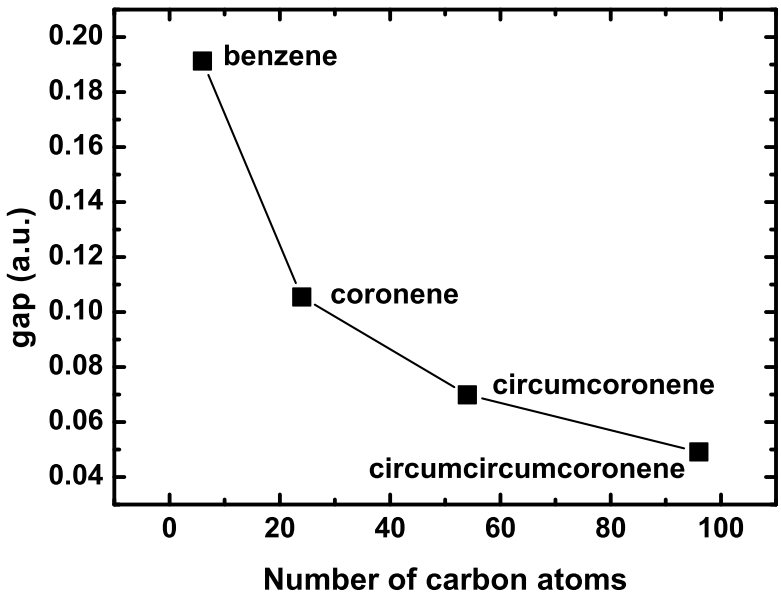

Figure 1: Magnitude of the HOMO-LUMO gap for benzene, coronene, circumcoronene, and circumcircumcoronene with the PBE functional and the co-r basis set (co-r** for circumcircumcoronene).