Supplementary Material for PCCP

Supporting Information for

Shannon Entropy as a New Measure of Aromaticity;

Shannon Aromaticity

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Table S1. Calculated charge densities at the bond critical points for the considered five-membered heterocycles using B3LYP and different basis sets.

Molecule	ρ_1	ρ_2	ρ_3	S_t
*6-31G***				
1a	0.2949263	0.2949583	0.2949058	1.0986123
1b	0.3199127	0.2913055	0.3199127	1.0976583
1c	0.3237686	0.2917469	0.3237648	1.0974363
1d	0.3326668	0.2850599	0.3326726	1.0960576
1e	0.3313751	0.2786796	0.3313752	1.0954155
1f	0.3380691	0.2722103	0.3380691	1.0936654
1g	0.3340243	0.2591229	0.3340240	1.0918871
1h	0.3397677	0.2528541	0.3397634	1.0896116
1i	0.3422694	0.2314297	0.3422946	1.0832530
*6-31+G***				
1a	0.2952842	0.2952730	0.2952856	1.0986122
1b	0.3195893	0.2915012	0.3195894	1.0976918
1c	0.3230385	0.2921129	0.3230385	1.0975132
1d	0.3324209	0.2851856	0.3324225	1.0960959
1e	0.3303926	0.2793554	0.3303934	1.0956073
1f	0.3371399	0.2729492	0.3371411	1.0939047
1g	0.3335039	0.2599044	0.3335039	1.0921189
1h	0.3393410	0.2532261	0.3393410	1.0897698
1i	0.3421025	0.2316377	0.3425998	1.0833042
*6-311++G***				
1a	0.2919120	0.2919856	0.2919129	1.0986123
1b	0.3169829	0.2880551	0.3169827	1.0976172
1c	0.3205634	0.2889963	0.3205616	1.0974468
1d	0.3299137	0.2815815	0.3299133	1.0959277
1e	0.3282699	0.2758066	0.3282709	1.0953812
1f	0.3349566	0.2692779	0.3349567	1.0935950
1g	0.3309741	0.2560547	0.3309737	1.0917465
1h	0.3369427	0.2491689	0.3369378	1.0892385

1i	0.3401166	0.2285123	0.3400893	1.0827845

Table S2. Calculated charge densities at the bond critical points for the considered mono-substituted benzene B3LYP/6-31+G**.

Mol.	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	S_t
2a	0.3011005	0.3170259	0.3102875	0.3102825	0.3170295	0.3010886	1.7915365
2b	0.3084472	0.3153697	0.3085326	0.3119742	0.3129592	0.3137294	1.7917254
2c	0.3060958	0.3136931	0.3115155	0.3114974	0.3137113	0.3060498	1.7917060
2d	0.3103605	0.3198025	0.3198557	0.3197337	0.3199399	0.3102952	1.7916590
2e	0.3121609	0.3121788	0.3108076	0.3144129	0.3078800	0.3075935	1.7917288
2f	0.3139997	0.3111726	0.3116084	0.3131317	0.3081406	0.3091286	1.7917376
2g	0.3083277	0.3092987	0.3136287	0.3112754	0.3115642	0.3128716	1.7917417
2h	0.3094927	0.3077029	0.3147622	0.3098547	0.3118078	0.3126052	1.7917321
2i	0.3092082	0.3113173	0.3130900	0.3118405	0.3130924	0.3091386	1.7917459
2j	0.3094052	0.3074619	0.3119020	0.3119179	0.3113550	0.3135450	1.7917393
2k	0.3050685	0.3134185	0.3112633	0.3112121	0.3134723	0.3049674	1.7916930
2l	0.3143586	0.3117501	0.3098967	0.3115277	0.3093869	0.3129783	1.7917458
2m	0.3109584	0.3075998	0.3131313	0.3089704	0.3134394	0.3121007	1.7917354
2n	0.3110768	0.3111891	0.3110985	0.3111909	0.3110727	0.3112120	1.7917590
2o	0.3109687	0.3119774	0.3110091	0.3118699	0.3088043	0.3097202	1.7917528
2p	0.3078949	0.3115084	0.3105615	0.3105487	0.3115217	0.3078841	1.7917472

Table S3. Calculated charge densities at the bond critical points for the considered penta and heptafulvens using B3LYP/6-31+G**.

Molecule	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	S_t
3a	0.2549986	0.3439377	0.3439390			1.0893908
3b	0.2578935	0.3440583	0.3440583			1.0900264
3c	0.2641675	0.3398469	0.3404877			1.0919407
3d	0.2704177	0.3348629	0.3348630			1.0937942
3e	0.2838875	0.3133782	0.3133782			1.0975516
4a	0.3231962	0.3007018	0.3247339	0.3007007	0.3231936	1.6087909
4b	0.3296703	0.2913183	0.3291079	0.2913120	0.3296710	1.6076515
4c	0.3321442	0.2871071	0.3318059	0.2872624	0.3316172	1.6069832
4d	0.3329813	0.2829435	0.3337439	0.2829434	0.3329813	1.6063048
4e	0.3326897	0.2670921	0.3345502	0.2670889	0.3326922	1.6037527

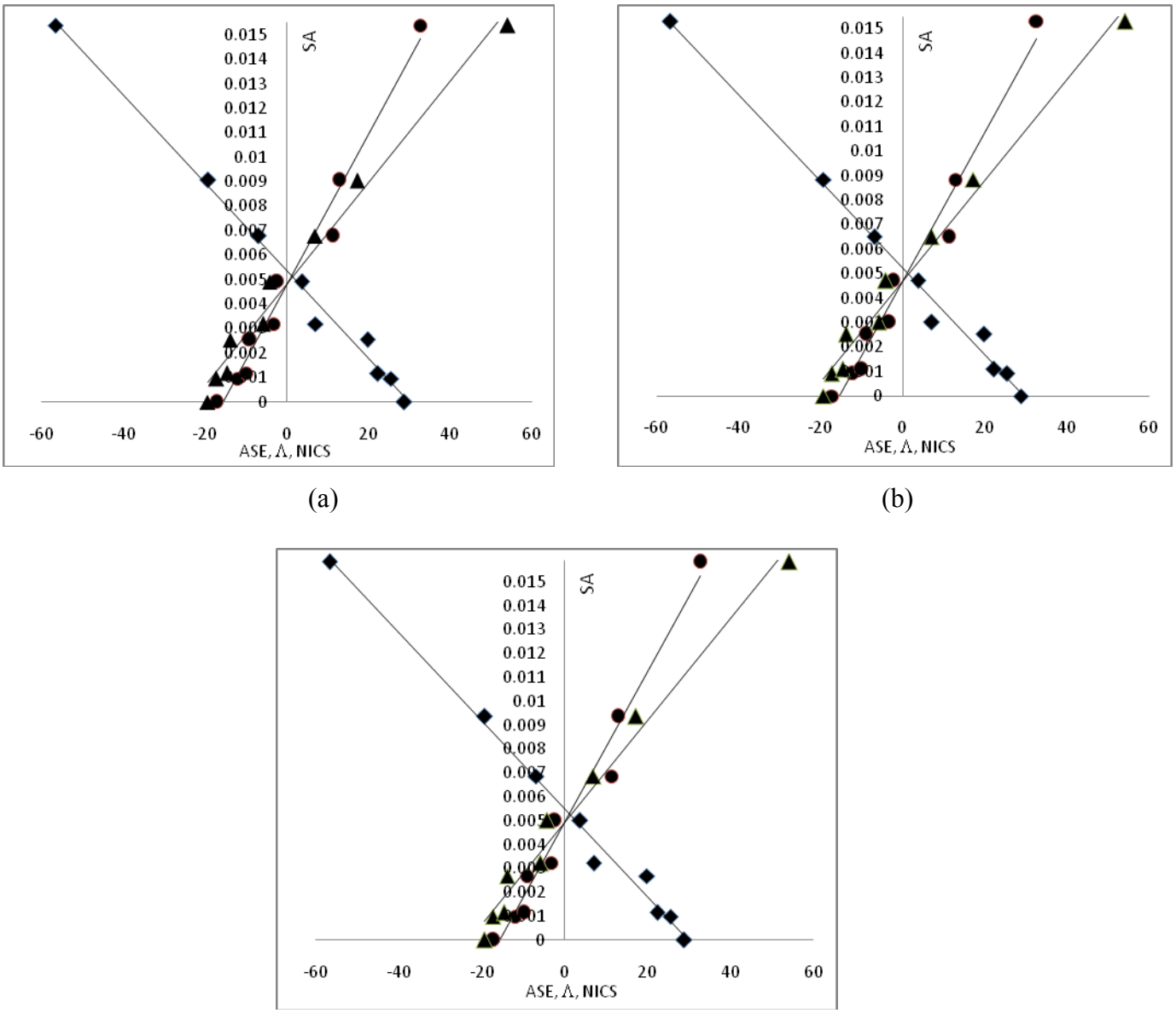
Table S4. Calculated charge densities at the bond critical points for the considered nonbenzeneoid, linear and angular polyacenes using B3LYP/6-31+G**.

Mol.	Ring	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	S_t
5a		0.3124118	0.3124344	0.3124485	0.3124660	0.3124137		1.6094379
5b		0.3356654	0.2837382	0.3258612	0.2837382	0.3356642		1.6064412
5c		0.3190933	0.3196678	0.2613566	0.3375398	0.2613963		1.6036452
6		0.3462339	0.2205383	0.3462339	0.2205381			1.3614967
7		0.2862889	0.2674065	0.3334868	0.2603433	0.3315021		1.6039234
8		0.3065059	0.3122805	0.3115651	0.3115711	0.3122755	0.3065123	1.7917251
9		0.3064771	0.3127034	0.3120903	0.3102010	0.3138603	0.3045050	1.7916993
10	a	0.3065282	0.3269818	0.2875762	0.3198718	0.2875764	0.3269829	1.7902795
	b	0.3065282	0.2428456	0.3378909	0.2428463			1.3757226
11	a	0.3071756	0.3214131	0.2968410	0.3137593	0.2968418	0.3214137	1.7912127
	b	0.3071756	0.2487357	0.3071735	0.2487283			1.3807580
12	a	0.3034482	0.3333023	0.3004527	0.3322503	0.3010271	0.3360024	1.9431280
	b	0.2678329	0.3150717	0.2854873	0.3203845	0.2797562		1.6070116
13	a	0.2999931	0.3222743	0.2986118	0.2934059	0.2986214	0.3222825	1.7910224
14	a	0.2949747	0.3260913	0.2938479	0.2873180	0.2938482	0.3260931	1.7903812
	b	0.2873180	0.3096525	0.3096560	0.2873239	0.3096518	0.3096472	1.7911476
15	a	0.2925353	0.3277951	0.2918001	0.2838212	0.2917946	0.3278145	1.7899979
	b	0.2838212	0.3139928	0.3042768	0.2835855	0.3042869	0.3140103	1.7908715
16	a	0.2914460	0.3285811	0.2908627	0.2820945	0.2908475	0.3285837	1.7898019
	b	0.2820945	0.3159741	0.3016963	0.2813439	0.3016952	0.3159917	1.7906567
	c	0.2813439	0.3084737	0.3084734	0.2813474	0.3084813	0.3084829	1.7908376
17	a	0.3185556	0.3051958	0.3202422	0.3021090	0.2967885	0.3011944	1.7913437
	b	0.2793065	0.2967890	0.2913451	0.3323622	0.2913447	0.2967885	1.7902708
18	a	0.2899068	0.2958618	0.2963788	0.2958708	0.2899120	0.3309119	1.7913114
	b	0.2956177	0.2958629	0.3076680	0.3182442	0.3182368	0.3076729	1.7906684
19	a	0.2965128	0.2993180	0.3195003	0.3041468	0.3214067	0.3011841	1.7912541
	b	0.2965128	0.2816100	0.3011094	0.2928151	0.3297810	0.2962217	1.7905698
20	a	0.3195642	0.3081686	0.3195171	0.3047945	0.2996324	0.3047614	1.7914597
	b	0.2635926	0.2635136	0.2996590	0.2631036	0.2996066	0.2996324	1.7910942
21	a	0.2969682	0.3243125	0.2959118	0.2913879	0.2958224	0.3244183	1.7911515
	b	0.2913879	0.3054666	0.3128204	0.2880080	0.3133259	0.3074861	1.7903572
22	a	0.3192003	0.3063447	0.3175018	0.3024552	0.2974587	0.3032042	1.7914265
	b	0.2974587	0.2771710	0.2929197	0.2899644	0.3335132	0.2893830	1.7900490
	c	0.2929197	0.3105614	0.3090641	0.2929192	0.3105680	0.3090692	1.7914125
23	a	0.2978288	0.3236252	0.2967692	0.2924090	0.2966964	0.3237177	1.7908339
	b	0.2924090	0.3039139	0.3146642	0.2884750	0.3149180	0.3059173	1.7912056
	c	0.2884749	0.2720262	0.2884823	0.2864439	0.3360758	0.2864354	1.7894789
24	a	0.2969682	0.3243125	0.2959118	0.2913879	0.2958224	0.3244183	1.7907231
	b	0.2913879	0.3054666	0.3128204	0.2880080	0.3133259	0.3074861	1.7912222
	c	0.2880080	0.2754128	0.2977311	0.2883647	0.3344214	0.2887657	1.7898275
	d	0.2977311	0.3038210	0.3186195	0.3070386	0.3168471	0.3030847	1.7914621
25	a	0.3090508	0.3185187	0.3025309	0.2992199	0.3025391	0.3185120	1.7914464
	b	0.2992199	0.2746091	0.2969949	0.2910083	0.2970005	0.2746068	1.7911054
	c	0.2910083	0.2948482	0.2910898	0.3330696	0.2910934	0.2948476	1.7905084
	d	0.2948475	0.2900051	0.3082463	0.3113761	0.3169271	0.3076281	1.7912836
26	a	0.2973116	0.3239500	0.2964331	0.2953191	0.2964324	0.3239431	1.7908616
	b	0.2953191	0.3059425	0.3135602	0.2895883	0.3135467	0.3059373	1.7913308

	c	0.2895882	0.2617761	0.3003298	0.2627284	0.3003255	0.2637269	1.7907945
	d	0.3028575	0.3003255	0.3027167	0.3180471	0.3099879	0.3180939	1.7914825

Table S4. Continued.

Mol.	Ring	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5	ρ_6	S_t
27	a	0.2936547	0.3269824	0.2928172	0.2851832	0.2927396	0.3269867	1.7901761
	b	0.2851832	0.3119334	0.3067139	0.2868697	0.3064771	0.3120701	1.7910642
	c	0.2868697	0.3002268	0.3172315	0.2836793	0.3174027	0.3024327	1.7908094
	d	0.2836793	0.2736769	0.2983186	0.2867338	0.3354403	0.2878004	1.7895609
	e	0.2983187	0.3045890	0.3178893	0.3077774	0.3161976	0.3037601	1.7915067
28	a	0.3016278	0.3211470	0.2980038	0.2925944	0.2977776	0.3235862	1.7909906
	b	0.2925944	0.2869778	0.3003904	0.2885804	0.3193175	0.3024195	1.7910937
	c	0.2885804	0.2943004	0.2947034	0.2878582	0.3338247	0.2875639	1.7902915
	d	0.2920429	0.3284498	0.2950193	0.2972018	0.2943004	0.3003904	1.7909246
	e	0.3003904	0.2947034	0.3105062	0.3095790	0.3159371	0.3044735	1.7914979
29	a	0.3186033	0.3088776	0.3184457	0.2996117	0.2973387	0.3022631	1.7913744
	b	0.3186422	0.3023805	0.2996668	0.3012579	0.3186013	0.3084447	1.7914339
	c	0.2780506	0.2973387	0.2757766	0.3063427	0.2764086	0.2996668	1.7908252
	d	0.3063427	0.2809893	0.2939971	0.2982846	0.3294054	0.2933996	1.7905304
	e	0.2939972	0.3005845	0.3219021	0.3039267	0.3196505	0.2965182	1.7911341



(a) (b)

(c)

Fig. S1. Correlation of SA with ASE (■), Λ (●) and NICS (▲) using: a) B3LYP/6-31G** b) B3LYP/6-31+G** c) B3LYP/6-311++G** levels of theory.

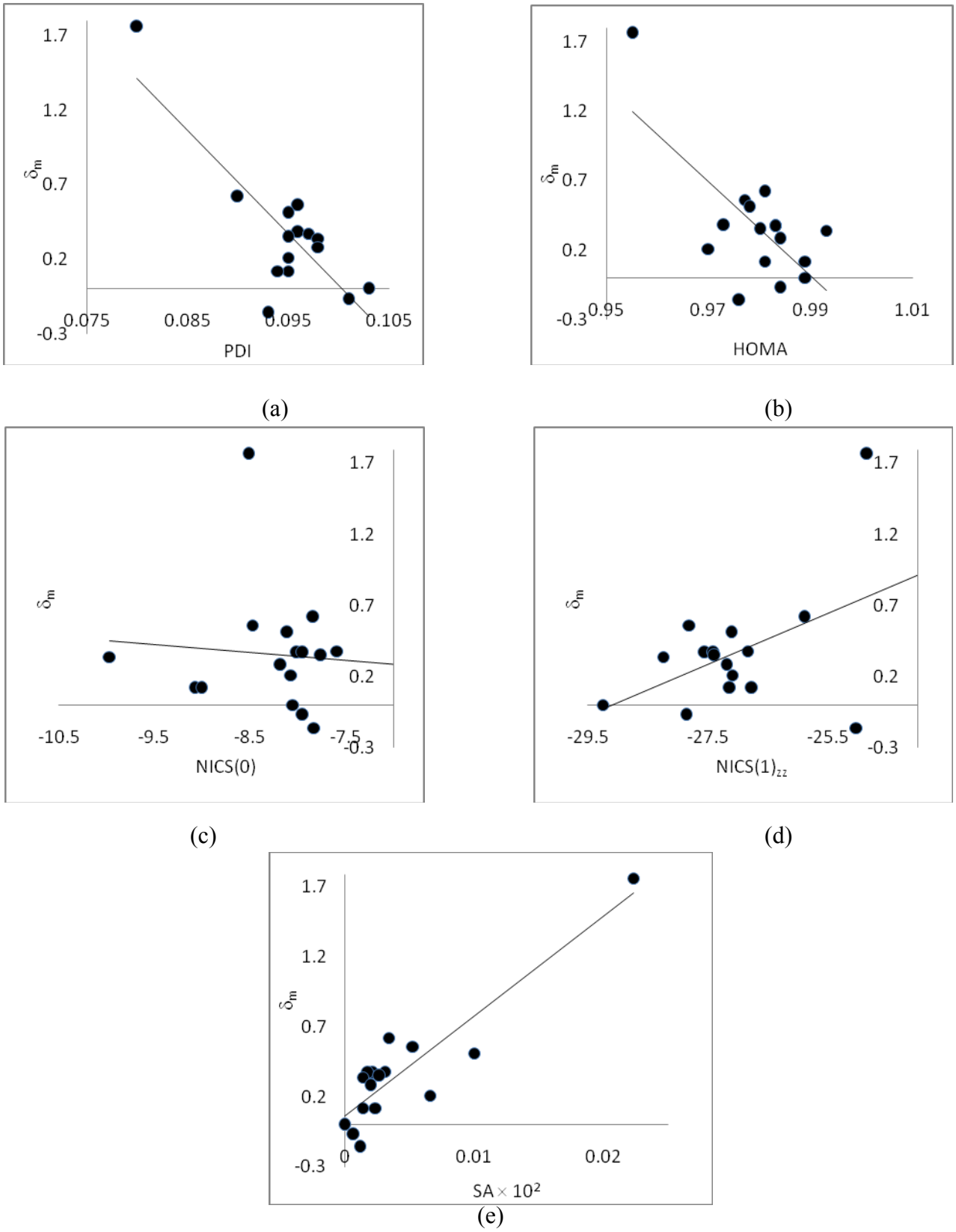


Fig. S2. Correlation of Hammett substitution constants with a) PDI, b) HOMA c) NICS(0), d) $NICS(1)_{zz}$ and e) SA indices.