Supporting information

One-electron and two-electron bond properties of all the studied molecules along with bond length. This table corresponds to Fig. 1 of the paper.

Molecule	wfn No		δ(C,C')	bond length	ρ_{bcp}	ε	$\nabla^2\rho_{bcp}$	G_{bcp}	V_{bcp}	$H_{bcp}= G_{bcp}+V_{bcp}$
Ethane	x	x	0.9912	1.5268	0.2530	0.0000	-0.6661	0.0505	-0.2676	-0.2171
Ethylene	x	x	1.8896	1.3165	0.3644	0.4485	-1.1983	0.1410	-0.5815	-0.4406
Cyclohexane	x	x	0.9612	1.5317	0.2551	0.0046	-0.6719	0.0514	-0.2707	-0.2194
Cyclohexene	1	2	1.8109	1.3208	0.3630	0.4744	-1.1729	0.1421	-0.5775	-0.4354
Cyclohexene	2	3	0.9956	1.5087	0.2646	0.0355	-0.7239	0.0540	-0.2890	-0.2350
Cyclohexene	3	4	0.9593	1.5310	0.2551	0.0053	-0.6734	0.0510	-0.2703	-0.2193
Cyclohexene	4	5	0.9616	1.5291	0.2562	0.0062	-0.6768	0.0518	-0.2729	-0.2210
Cyclohexdiene	2	3	1.0635	1.4749	0.2802	0.0808	-0.8015	0.0599	-0.3202	-0.2603
Cyclohexdiene	3	4	1.7739	1.3240	0.3622	0.4429	-1.1760	0.1385	-0.5711	-0.4325
Cyclohexdiene	4	5	0.9925	1.5107	0.2639	0.0350	-0.7205	0.0537	-0.2875	-0.2338
Cyclohexdiene	5	6	0.9594	1.5329	0.2541	0.0051	-0.6691	0.0504	-0.2680	-0.2176
Benzene	x	x	1.3878	1.3859	0.3274	0.2306	-1.0163	0.0965	-0.4471	-0.3506
Naphthalene	1	6	1.2216	1.4204	0.3095	0.1595	-0.9320	0.0799	-0.3927	-0.3129
Naphthalene	5	6	1.5330	1.3580	0.3432	0.3052	-1.0913	0.1127	-0.4983	-0.3855
Naphthalene	5	4	1.2452	1.4163	0.3106	0.1651	-0.9386	0.0815	-0.3976	-0.3161
Naphthalene	1	2	1.2784	1.4091	0.3170	0.1893	-0.9598	0.0873	-0.4146	-0.3273
Tetralene	1	5	1.3473	1.3940	0.3234	0.2248	-0.9899	0.0941	-0.4357	-0.3416
Tetralene	5	6	1.4113	1.3795	0.3307	0.2465	-1.0320	0.0997	-0.4575	-0.3577
Tetralene	6	4	1.3656	1.3877	0.3263	0.2233	-1.0127	0.0952	-0.4436	-0.3484
Tetralene	1	2	1.3711	1.3927	0.3238	0.2465	-0.9800	0.0975	-0.4400	-0.3425
Tetralene	1	7	0.9800	1.5188	0.2608	0.0353	-0.7048	0.0523	-0.2807	-0.2285
Tetralene	7	9	0.9624	1.5279	0.2567	0.0067	-0.6807	0.0516	-0.2734	-0.2218
Tetralene	9	10	0.9620	1.5266	0.2575	0.0043	-0.6828	0.0523	-0.2754	-0.2230
Anthracene	2	4	1.3468	1.3894	0.3262	0.2247	-1.0086	0.0947	-0.4416	-0.3469
Anthracene	4	14	1.1650	1.4359	0.3014	0.1319	-0.8963	0.0733	-0.3706	-0.2973
Anthracene	14	22	1.5980	1.3473	0.3494	0.3399	-1.1207	0.1199	-0.5199	-0.4000
Anthracene	22	18	1.1846	1.4324	0.3020	0.1367	-0.8995	0.0747	-0.3742	-0.2995
Anthracene	4	6	1.2140	1.4246	0.3086	0.1587	-0.9220	0.0802	-0.3908	-0.3107
Phenanthrene	1	3	1.6304	1.3386	0.3549	0.3591	-1.1521	0.1249	-0.5378	-0.4129
Phenanthrene	3	6	1.1431	1.4404	0.2993	0.1212	-0.8885	0.0712	-0.3646	-0.2934
Phenanthrene	6	8	1.3085	1.4044	0.3191	0.2093	-0.9657	0.0902	-0.4218	-0.3316
Phenanthrene	8	7	1.1183	1.4612	0.2880	0.1180	-0.8253	0.0658	-0.3378	-0.2721
Phenanthrene	6	22	1.2702	1.4084	0.3160	0.1847	-0.9608	0.0856	-0.4113	-0.3258
Phenanthrene	22	18	1.4793	1.3656	0.3391	0.2767	-1.0745	0.1075	-0.4835	-0.3761
Phenanthrene	18	14	1.2963	1.4018	0.3188	0.1882	-0.9791	0.0877	-0.4203	-0.3325
Phenanthrene	14	10	1.4763	1.3676	0.3376	0.2768	-1.0641	0.1069	-0.4797	-0.3729
Phenanthrene	10	8	1.2755	1.4106	0.3137	0.1878	-0.9450	0.0854	-0.4071	-0.3217
Chrysene	3	5	1.3776	1.3924	0.3251	0.2506	-0.9881	0.0972	-0.4413	-0.3442
Chrysene	5	6	1.1740	1.4352	0.3010	0.1386	-0.8899	0.0744	-0.3712	-0.2968
Chrysene	6	4	1.5936	1.3437	0.3519	0.3389	-1.1373	0.1213	-0.5268	-0.4056
Chrysene	4	2	1.1707	1.4288	0.3057	0.1336	-0.9208	0.0752	-0.3807	-0.3054
Chrysene	2	1	1.3012	1.4044	0.3194	0.2039	-0.9691	0.0897	-0.4218	-0.3320
Chrysene	1	3	1.1453	1.4532	0.2919	0.1338	-0.8405	0.0689	-0.3480	-0.2791
Chrysene	2	16	1.2503	1.4125	0.3137	0.1746	-0.9512	0.0835	-0.4047	-0.3213
Chrysene	16	26	1.5001	1.3617	0.3414	0.2868	-1.0858	0.1098	-0.4910	-0.3812
Chrysene	26	25	1.2771	1.4062	0.3164	0.1787	-0.9682	0.0856	-0.4132	-0.3276

Molecule	wfn No		δ(C,C')	bond length	ρ_{bcp}	ε	$\nabla^2\rho_{bcp}$	G_{bcp}	V_{bcp}	$H_{bcp}=G_{bcp}+V_{bcp}$
Chrysene	25	15	1.4978	1.3641	0.3396	0.2873	-1.0737	0.1091	-0.4866	-0.3775
Chrysene	15	1	1.2548	1.4166	0.3104	0.1772	-0.9291	0.0828	-0.3979	-0.3151
Dibenz[a,j]anthracene	14	10	1.3512	1.3865	0.3282	0.2270	-1.0199	0.0959	-0.4468	-0.3509
Dibenz[a,j]anthracene	10	8	1.1260	1.4449	0.2969	0.1204	-0.8787	0.0692	-0.3582	-0.2889
Dibenz[a,j]anthracene	8	7	1.6509	1.3353	0.3570	0.3714	-1.1620	0.1273	-0.5452	-0.4178
Dibenz[a,j]anthracene	7	3	1.1253	1.4463	0.2962	0.1121	-0.8748	0.0690	-0.3567	-0.2877
Dibenz[a,j]anthracene	3	2	1.2852	1.4049	0.3179	0.1925	-0.9694	0.0873	-0.4170	-0.3297
Dibenz[a,j]anthracene	2	1	1.4629	1.3684	0.3375	0.2682	-1.0673	0.1057	-0.4782	-0.3725
Dibenz[a,j]anthracene	1	4	1.3118	1.3982	0.3208	0.1951	-0.9888	0.0894	-0.4261	-0.3366
Dibenz[a,j]anthracene	4	5	1.4598	1.3704	0.3360	0.2691	-1.0564	0.1052	-0.4744	-0.3693
Dibenz[a,j]anthracene	5	6	1.2912	1.4071	0.3155	0.1959	-0.9529	0.0872	-0.4126	-0.3254
Dibenz[a,j]anthracene	6	3	1.3115	1.4039	0.3193	0.2118	-0.9662	0.0905	-0.4226	-0.3321
Dibenz[a,j]anthracene	6	9	1.1002	1.4683	0.2844	0.1096	-0.8092	0.0634	-0.3291	-0.2657
Dibenz[a,j]anthracene	9	10	1.2492	1.4155	0.3134	0.1799	-0.9430	0.0843	-0.4044	-0.3201
Dibenz[a,j]anthracene	9	11	1.3563	1.3908	0.3243	0.2304	-0.9924	0.0952	-0.4386	-0.3433
Pyrene	1	2	1.3890	1.3838	0.3284	0.2354	-1.0211	0.0974	-0.4501	-0.3527
Pyrene	3	4	1.3411	1.3912	0.3252	0.2203	-1.0037	0.0940	-0.4389	-0.3449
Pyrene	4	5	1.2562	1.4113	0.3155	0.1816	-0.9546	0.0855	-0.4097	-0.3242
Pyrene	5	7	1.1750	1.4324	0.3040	0.1439	-0.9022	0.0759	-0.3773	-0.3014
Pyrene	8	9	1.1290	1.4460	0.2961	0.1130	-0.8738	0.0691	-0.3566	-0.2875
Pyrene	9	10	1.6464	1.3389	0.3543	0.3694	-1.1446	0.1256	-0.5374	-0.4118
Biphenyl (equilibrium)	1	2	1.0233	1.4911	0.2750	0.0555	-0.7787	0.0545	-0.3037	-0.2492
Biphenyl (equilibrium)	2	3	1.3541	1.3926	0.3237	0.2305	-0.9906	0.0949	-0.4374	-0.3425
Biphenyl (equilibrium)	3	5	1.3925	1.3844	0.3281	0.2339	-1.0199	0.0972	-0.4493	-0.3521
Biphenyl (equilibrium)	5	7	1.3858	1.3845	0.3280	0.2294	-1.0203	0.0967	-0.4486	-0.3518
Biphenyl (planar)	1	2	1.0366	1.5010	0.2683	0.0739	-0.7407	0.0533	-0.2918	-0.2385
Biphenyl (planar)	2	3	1.3503	1.3961	0.3218	0.2247	-0.9800	0.0934	-0.4317	-0.3384
Biphenyl (planar)	3	5	1.3955	1.3835	0.3286	0.2364	-1.0211	0.0978	-0.4509	-0.3531
Biphenyl (planar)	5	7	1.3839	1.3834	0.3292	0.2280	-1.0285	0.0971	-0.4514	-0.3543