Table 7 – Orbital energies (eV) from HOMO -10 to LUMO + 10

CBNs	HOMO – 10	HOMO – 9	HOMO – 8	HOMO – 7	HOMO – 6	HOMO – 5	HOMO – 4	HOMO – 3	HOMO – 2	HOMO – 1	HOMO	LUMO	LUMO + 1	LUMO + 2	LUMO + 3	LUMO + 4	LUMO + 5	LUMO + 6	LUMO + 7	LUMO + 8	LUMO + 9	LUMO + 10
Benzene	-16.1573	-14.0084	-12.4026	-11.8213	-11.2553	-11.2543	-9.6793	-9.1631	-9.1629	-6.6056	-6.6051	0.1887	0.1888	2.5595	4.0242	4.0243	4.5466	5.0337	5.0346	5.2644	8.3231	8.3246
Naphthalene	-11.1876	-11.1072	-10.7376	-10.3868	-9.8783	-9.0354	-8.8269	-8.6915	-7.5532	-6.4403	-5.6913	-0.8671	-0.0557	1.0672	2.6767	2.8908	3.1644	3.4015	4.6046	4.6516	4.8372	5.0619
Anthracene	-10.4152	-10.147	-9.639	-9.2853	-8.9731	-8.7286	-8.0714	-7.9366	-6.8092	-6.3593	-5.1292	-1.54	-0.1937	0.3283	1.333	1.9498	2.7927	2.8792	3.1051	3.9407	4.0714	4.358
Phenanthrene	-10.5288	-9.7393	-9.6344	-9.5705	-8.9022	-8.6625	-8.3729	-7.5511	-6.9624	-5.9373	-5.6336	-0.9015	-0.7283	0.3473	1.1207	2.3441	2.6233	2.9501	2.9761	4.1088	4.1146	4.1226
Pyrene	-9.8193	-9.7559	-9.6571	-9.1134	-8.7818	-8.5294	-7.914	-7.2742	-6.7752	-6.1075	-5.23	-1.3876	-0.5217	0.0544	0.696	1.7123	2.635	3.0187	3.205	3.2638	3.6693	4.1706
Chrysene	-9.5191	-9.244	-8.9123	-8.876	-8.5184	-8.4239	-7.4703	-7.2399	-6.3684	-5.9204	-5.4141	-1.1747	-0.7526	-0.3429	0.7616	0.8525	2.3816	2.6409	2.6924	2.8728	3.0583	3.5994
Benzanthracene	-9.5372	-9.1894	-9.0401	-8.8674	-8.6282	-8.1972	-7.6982	-7.1065	-6.5918	-5.8533	-5.2253	-1.4565	-0.802	0.0316	0.5159	1.2084	1.9212	2.6927	2.8154	2.8414	3.2928	3.5811
Tetracene	-9.7324	-9.0514	-9.0219	-8.9411	-8.6899	-8.1297	-7.6591	-7.3836	-6.3135	-6.2284	-4.76	-1.9845	-0.3265	-0.283	0.8778	1.3593	1.4317	2.8168	2.829	2.9503	3.3783	3.5808
Triphenylene	-9.6352	-9.6317	-9.6315	-8.6171	-8.6158	-7.7988	-7.4558	-7.4557	-6.2801	-5.7512	-5.7509	-0.8396	-0.8391	-0.587	0.9834	0.9841	1.5668	2.5765	2.7367	2.7369	3.7308	3.7316
Perylene	-9.4052	-9.3072	-8.5855	-8.5292	-8.5168	-8.4282	-6.7183	-6.7039	-6.6128	-6.4598	-4.8566	-1.7991	-0.3389	-0.0545	0.1241	0.1657	2.1928	2.3957	2.4475	2.9418	2.9761	3.4318
Benzo[a]pyrene	-9.217	-9.2137	-8.9727	-8.7689	-8.4573	-7.789	-7.3933	-6.7817	-6.6239	-5.9646	-5.0056	-1.6436	-0.7479	-0.0827	0.1229	0.866	1.403	2.6132	2.8329	2.9853	3.0452	3.423
Benzo[e]pyrene	-9.7148	-9.5158	-8.5747	-8.5303	-8.4921	-7.8147	-7.6328	-6.6403	-6.5467	-5.8198	-5.3149	-1.302	-0.8247	-0.263	-0.076	1.2107	1.5274	2.3232	2.5491	2.7554	2.9316	3.5394
Benzo[ghi]perylene	-9.4897	-8.6698	-8.5188	-8.5092	-8.4757	-7.8527	-6.8353	-6.8162	-6.6208	-5.7853	-5.1238	-1.5121	-0.8065	-0.1783	0.0938	0.2033	1.5214	2.3139	2.5345	2.6032	2.8766	2.9826
Coronene	-8.8314	-8.8299	-8.4504	-8.4465	-8.3617	-7.1749	-7.0929	-6.6665	-6.6647	-5.3912	-5.3884	-1.2067	-1.2046	-0.1691	-0.1677	0.3913	0.8218	1.9489	2.5912	2.8293	2.8303	2.9663