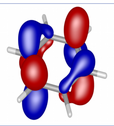
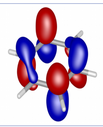
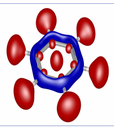
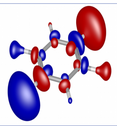
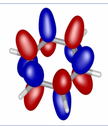
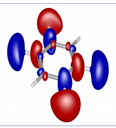
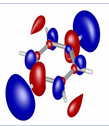
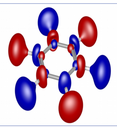
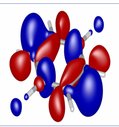
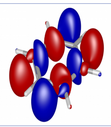
Table 6 – eON and LUMO to LUMO + 10 orbitals of all fourteen molecules B3LYP/6-31G*

CBNs	LUMO	LUMO + 1	LUMO + 2	LUMO + 3	LUMO + 4	LUMO + 5	LUMO + 6	LUMO + 7	LUMO + 8	LUMO + 9	LUMO + 10
	0.07776455	0.07775724	0.03517863	0.0203729	0.02035098	0.02015011	0.02014803	0.0197748	0.01875591	0.01632872	0.01632766
Benzene											
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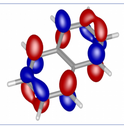
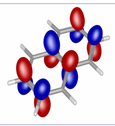
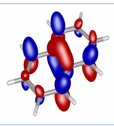
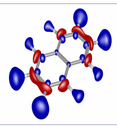
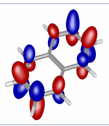
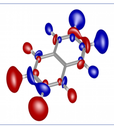
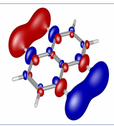
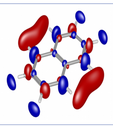
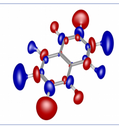
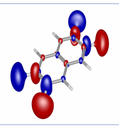
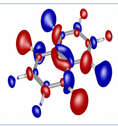
Naphthalene											
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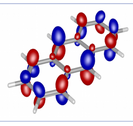
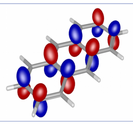
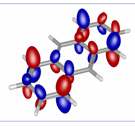
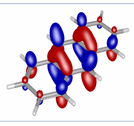
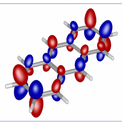
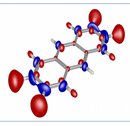
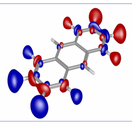
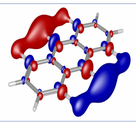
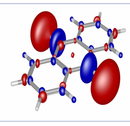
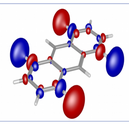
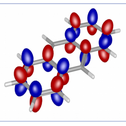
Anthracene											
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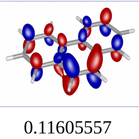
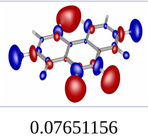
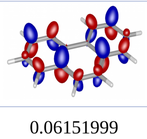
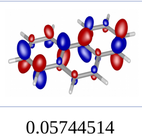
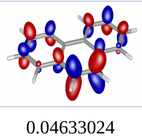
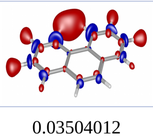
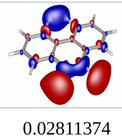
Phenanthrene											
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Pyrene											
	0.10282857	0.08283404	0.07575725	0.05871881	0.05440305	0.04017398	0.03413714	0.0235991	0.01971125	0.00589881	0.00520605
Chrysene											
	0.1295112	0.09248669	0.07399922	0.0620389	0.05153626	0.04378007	0.03269845	0.02258924	0.01825959	0.00348612	0.00325298
Benzanthracene											
	0.18243079	0.08354964	0.07257284	0.05532551	0.05036428	0.04552849	0.03322272	0.02441097	0.01961117	0.00879059	0.00823252
Tetracene											
	0.08822214	0.08765472	0.07545154	0.05430172	0.05396938	0.04916821	0.02596705	0.02590525	0.0201573	0.00628682	0.00494027
Triphenylene											
	0.13821737	0.06835748	0.06803926	0.06493864	0.06236636	0.04099378	0.03628066	0.03062568	0.02233793	0.01875896	0.00807564
Perylene											
	0.14809235	0.08774617	0.07233285	0.06402353	0.05620058	0.0489754	0.03205207	0.03036943	0.02129515	0.01613539	0.00320384
Benzo[a]pyrene											
	0.11032404	0.08608538	0.06958429	0.06674987	0.05260884	0.04726294	0.03824546	0.02522344	0.02396869	0.01776976	0.00525379
Benzo[e]pyrene											
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Benzo[ghi]perylene											
	0.09664436	0.09654481	0.06016839	0.05958061	0.05583118	0.053744	0.03802832	0.03180866	0.03175009	0.0203881	0.02027562
Coronene											