

Supplementary Information

Non-linear optical and electronic properties of oxa[n]circulenes:
A theoretical insight

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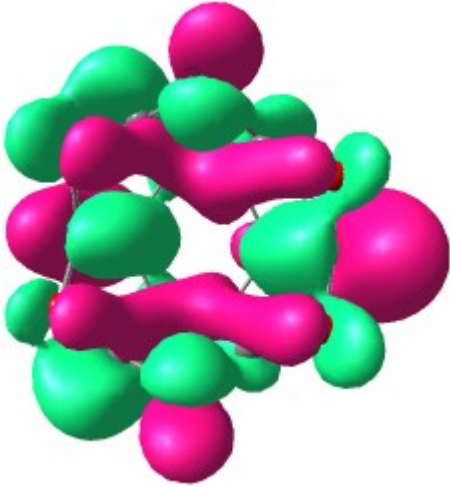
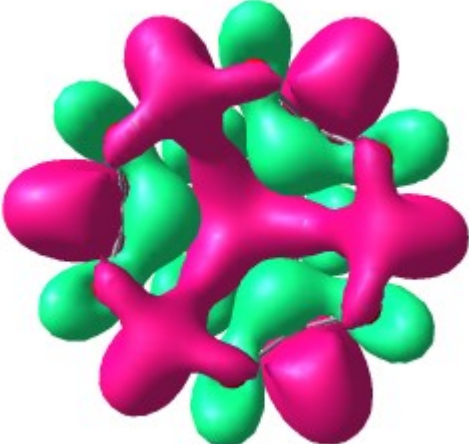
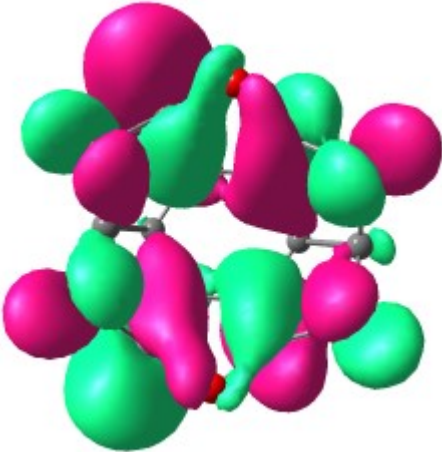
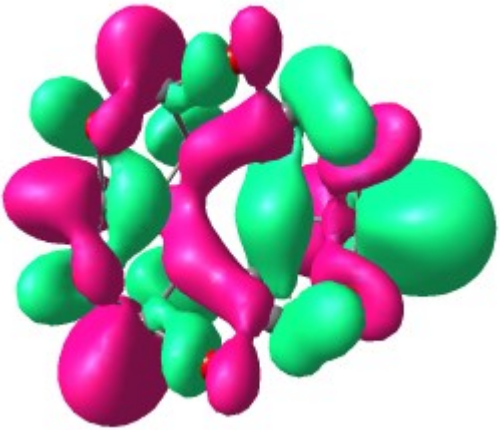
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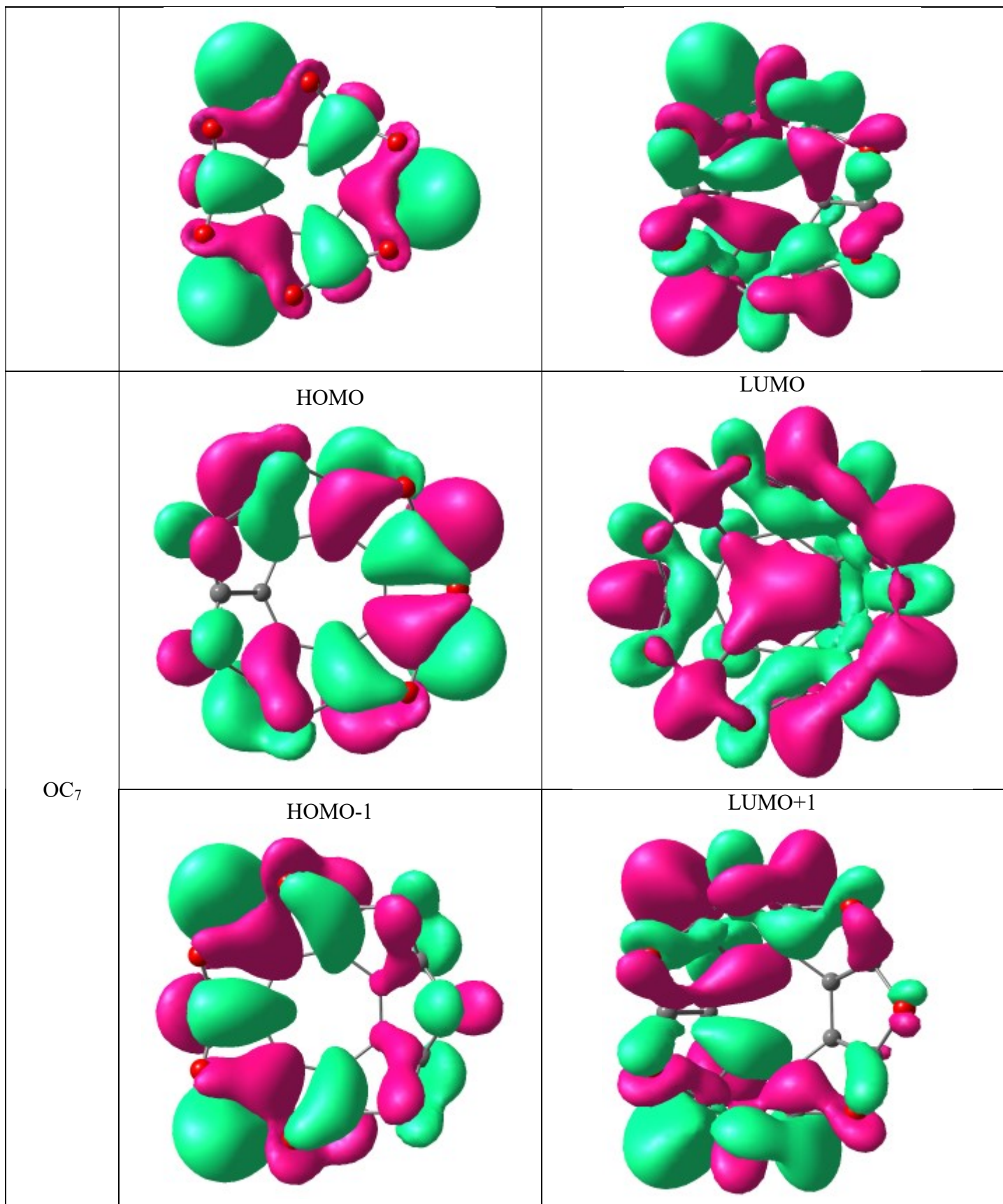
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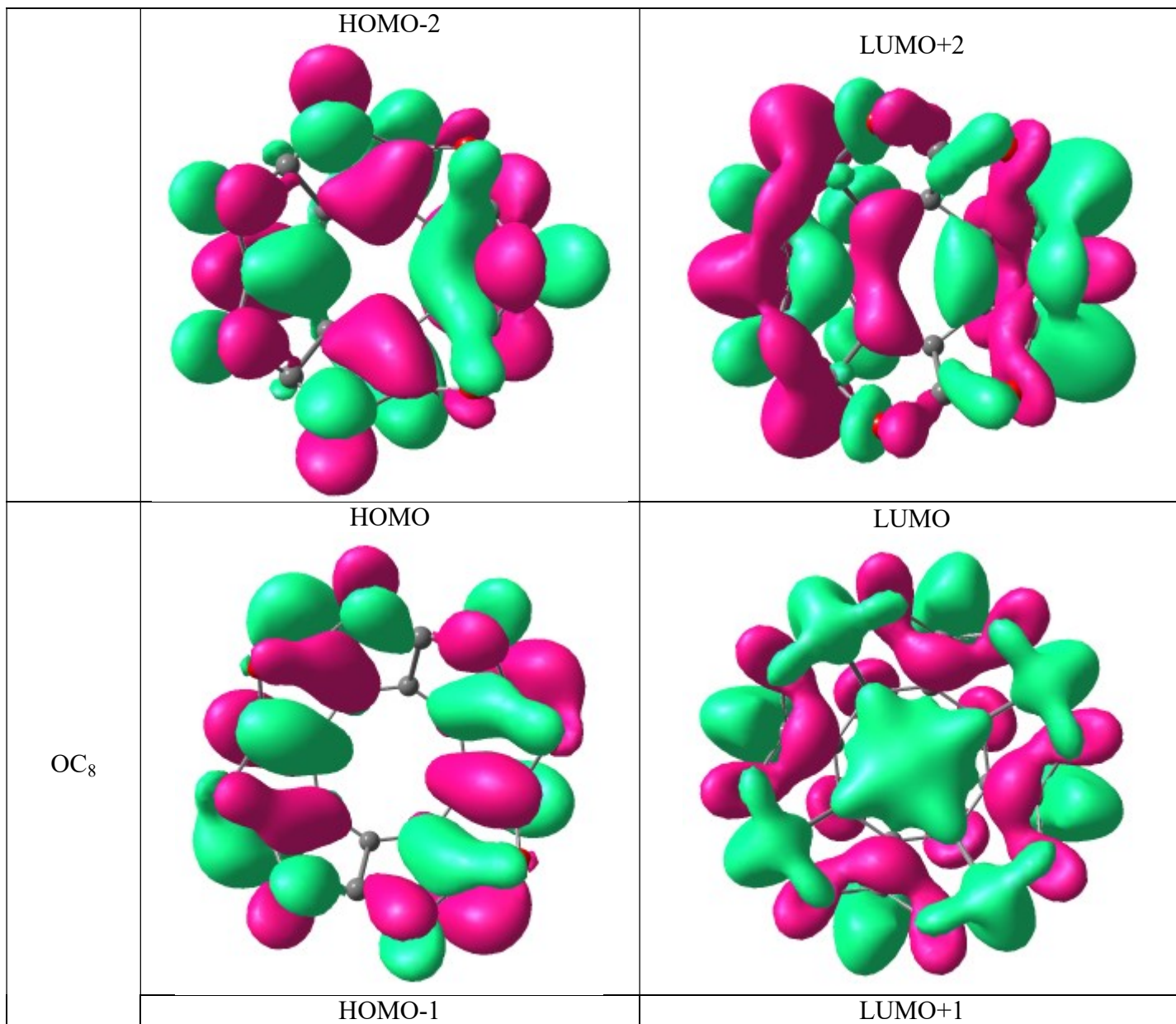
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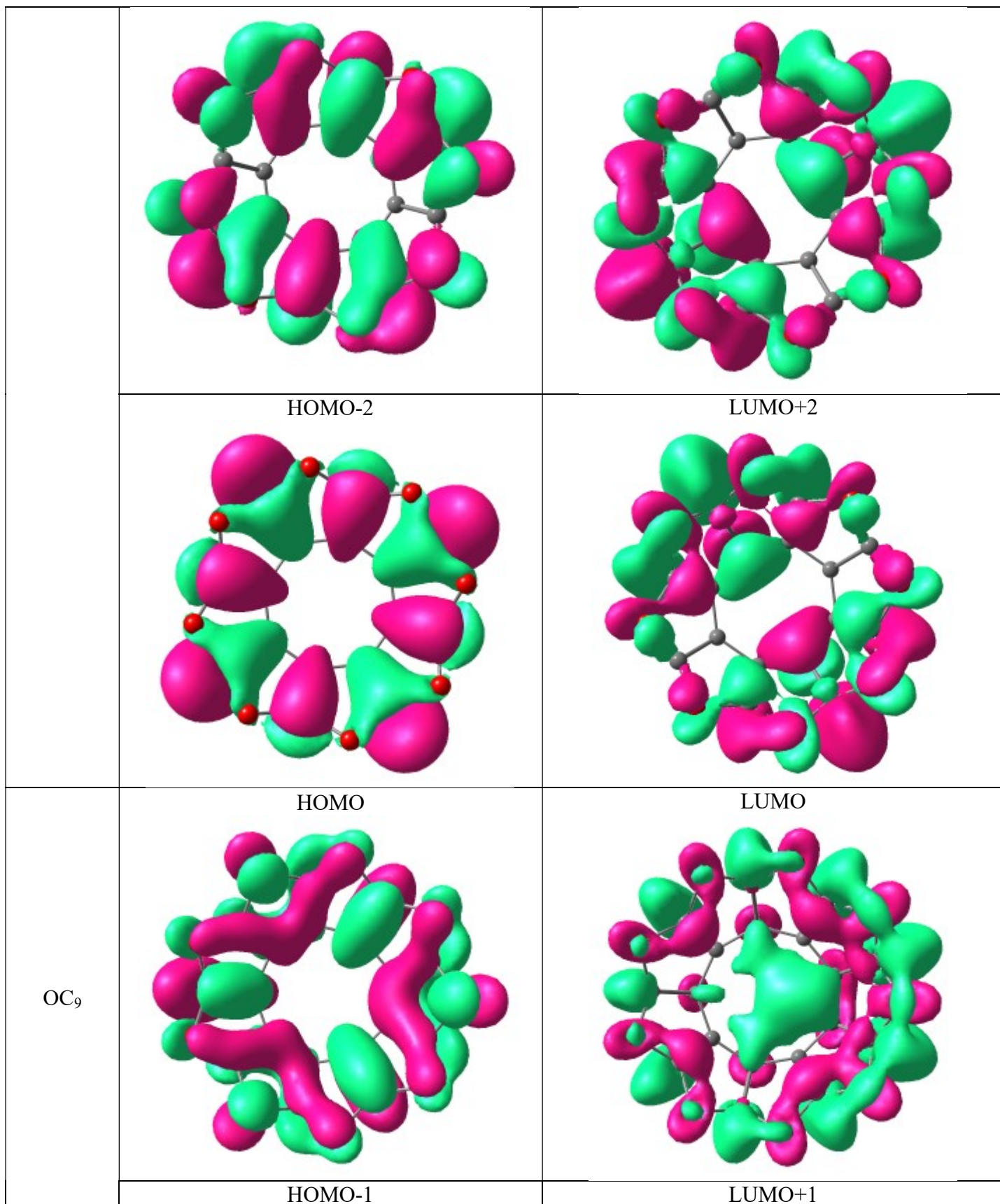
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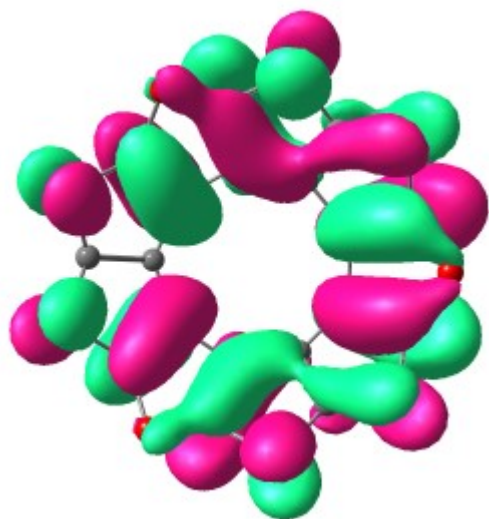
Table S1. Frontier molecular orbitals (FMOs)

Molecules	FMOs	
OC ₆	HOMO 	LUMO 
	HOMO-1 	LUMO+1 
	HOMO-2 	LUMO+2

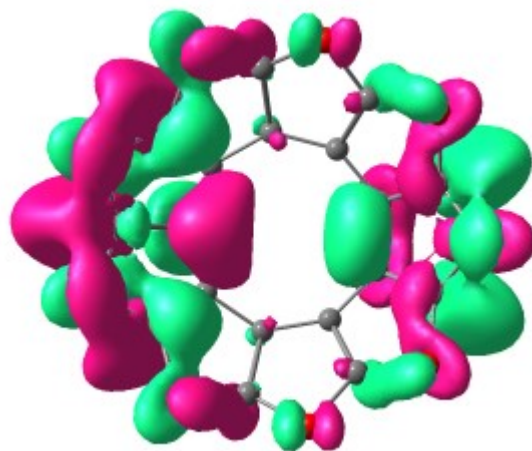




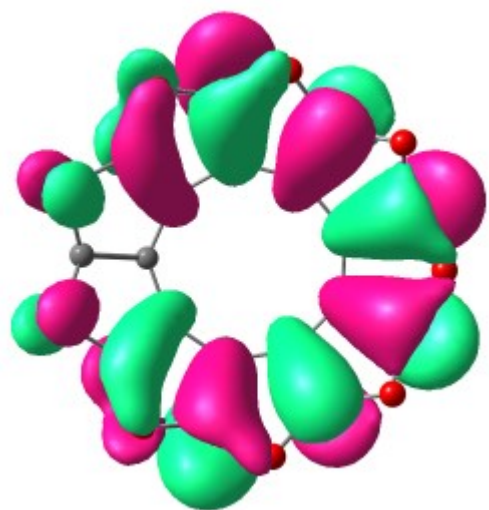




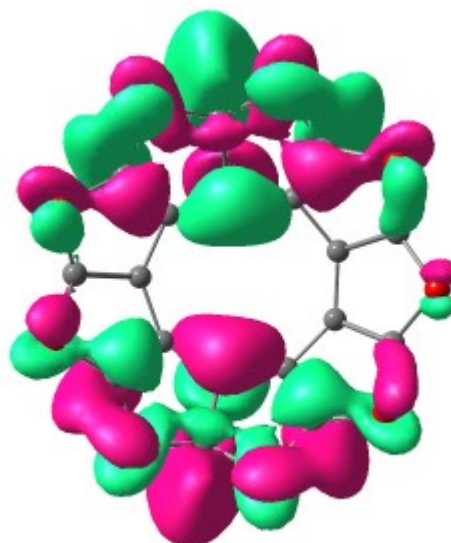
HOMO-2



LUMO+2

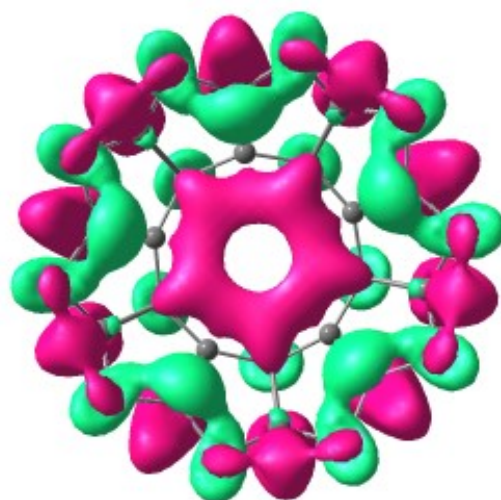
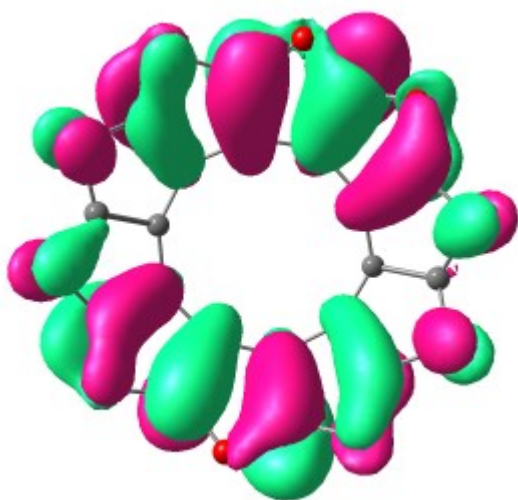


HOMO

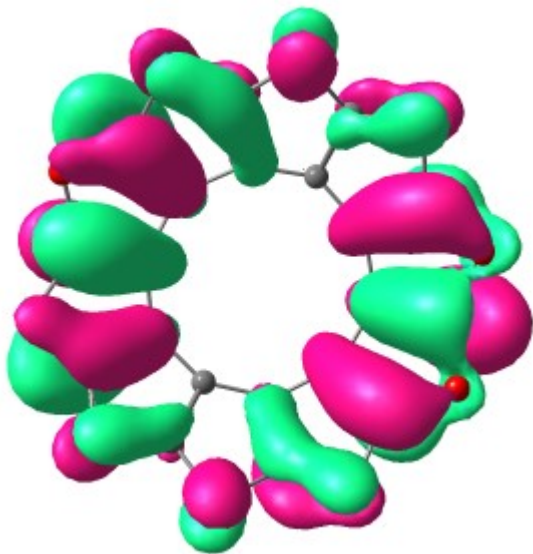


LUMO

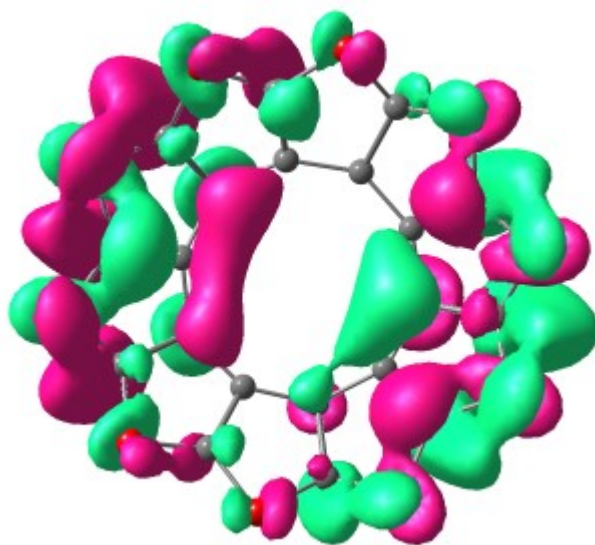
OC₁₀



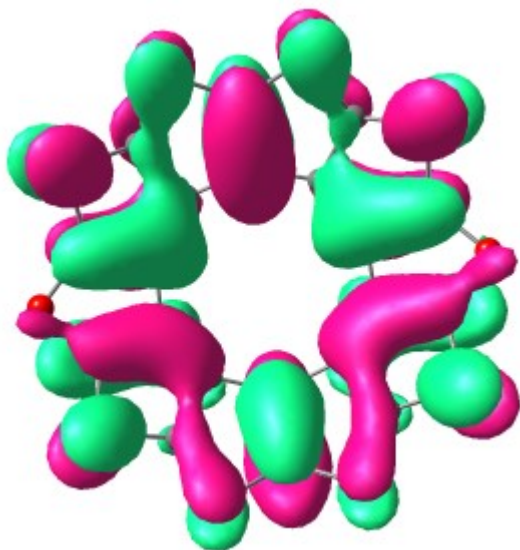
HOMO-1



LUMO+1



HOMO-2



LUMO+2

