Electronic Supporting Information

for

Toward an Understanding of Electronic Excitation Energies Beyond the Molecular Orbital Picture

P. Kimber, F. Plasser

December 31, 2019

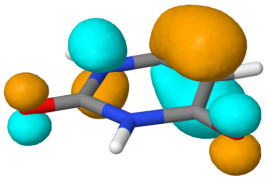
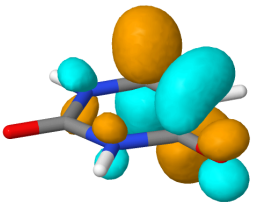
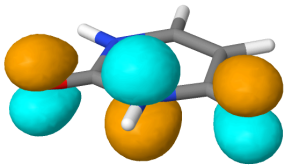
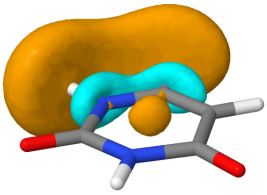
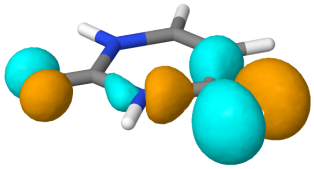
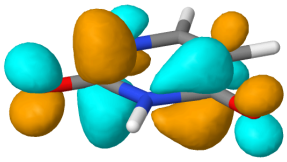
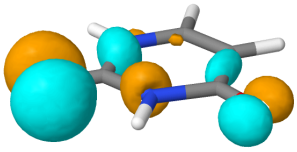
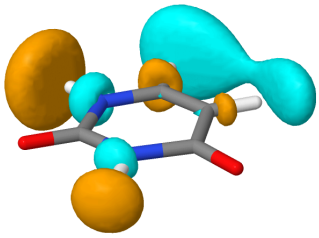
Occupied	Virtual
	
HOMO (-10.0 eV)	LUMO (2.7 eV)
	
HOMO-1 (-11.9 eV)	LUMO+1 (4.1 eV)
	
HOMO-2 (-12.2 eV)	LUMO+2 (4.8 eV)
	
HOMO-3 (-13.1 eV)	LUMO+3 (5.6 eV)

Figure S1 - frontier orbitals and energies of uracil computed at the Hartree-Fock/def2-SV(P) level.

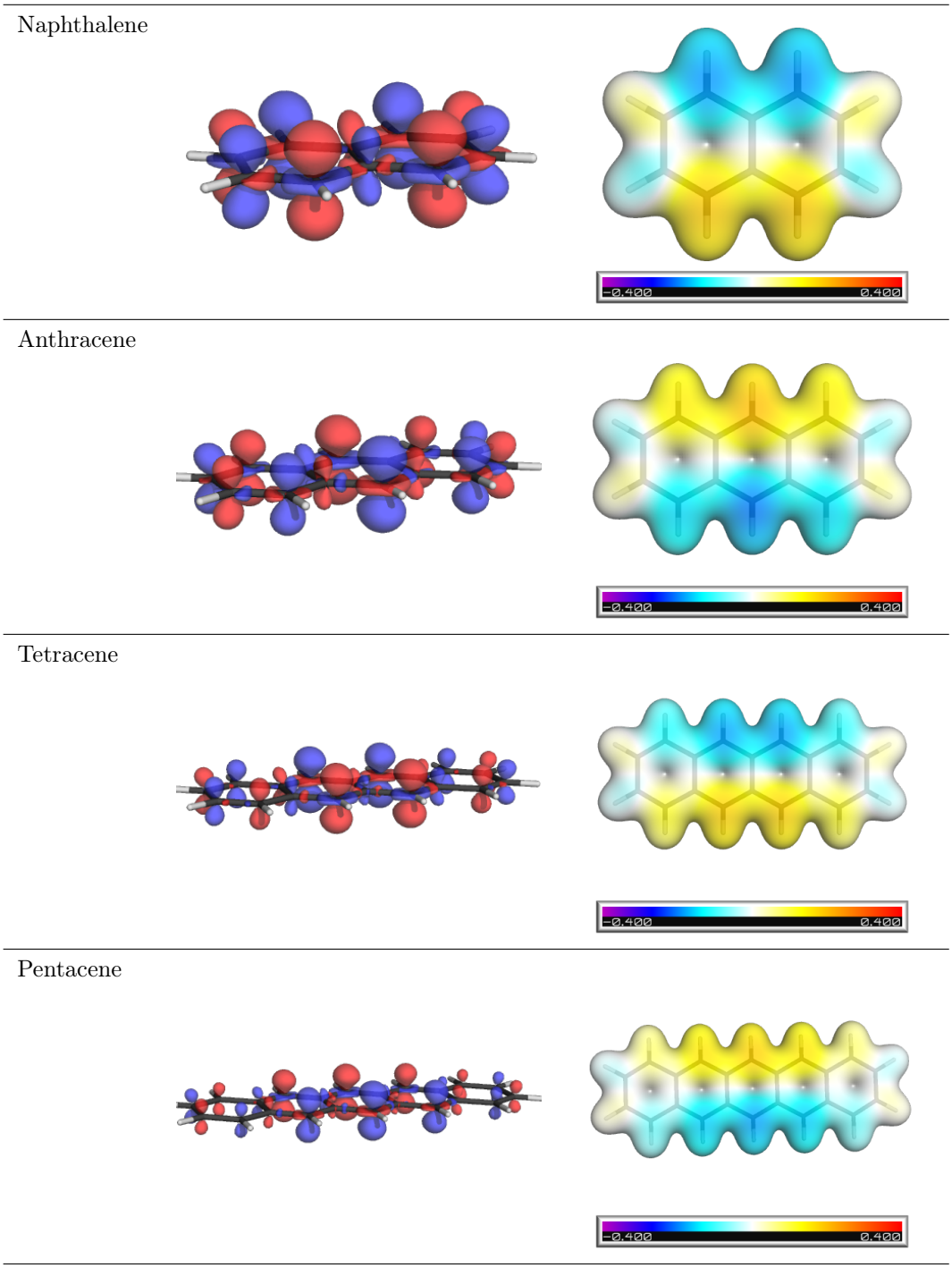


Figure S2 - transition densities and electrostatic potential maps of the singlet B_{2u} states computed for the polyacene systems at the ADC(2)/aug-cc-PVDZ level of theory.

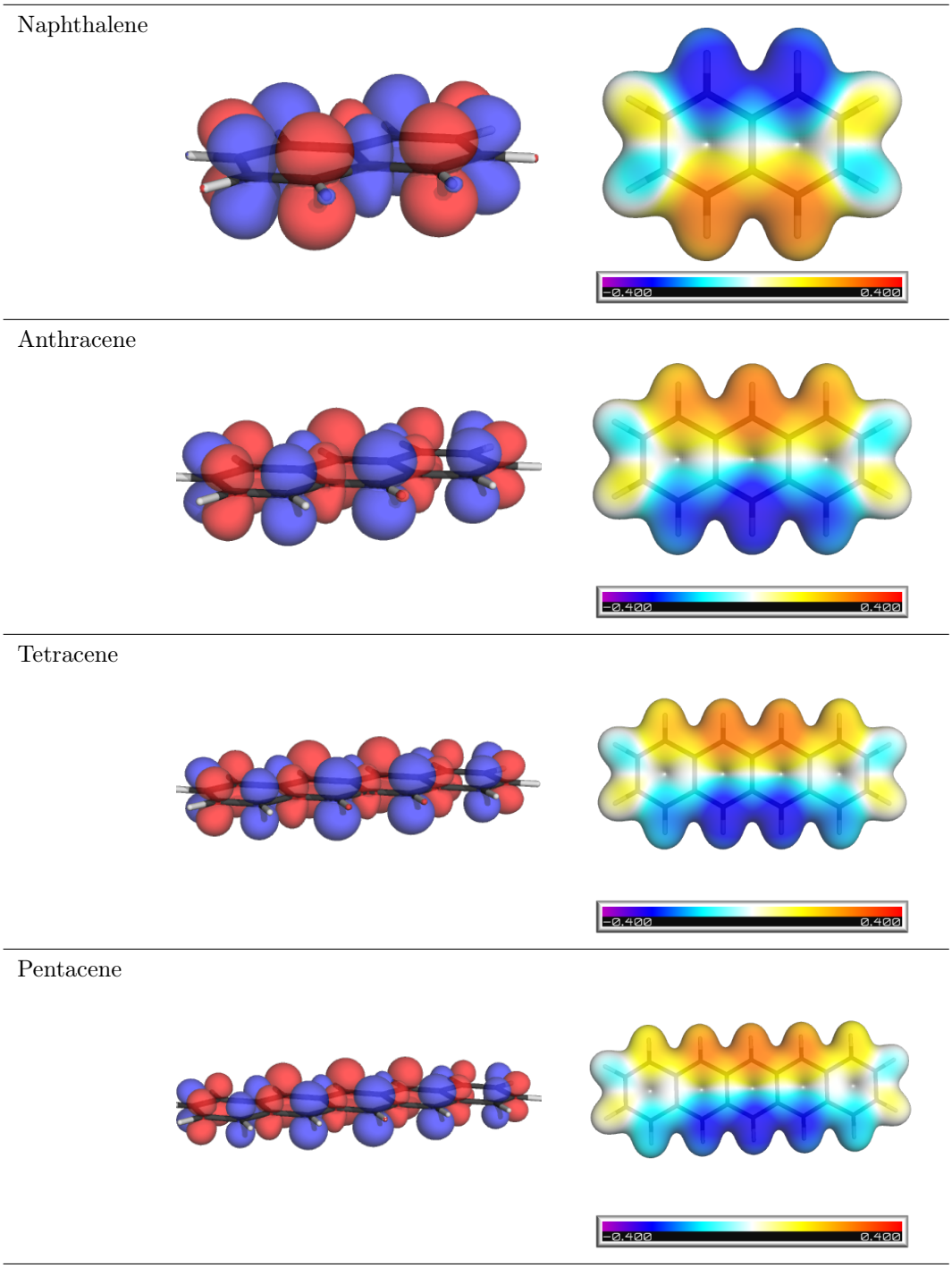


Figure S3 - transition densities and electrostatic potential maps of the triplet B_{2u} states computed for the polyacene systems at the ADC(2)/aug-cc-PVDZ level of theory.

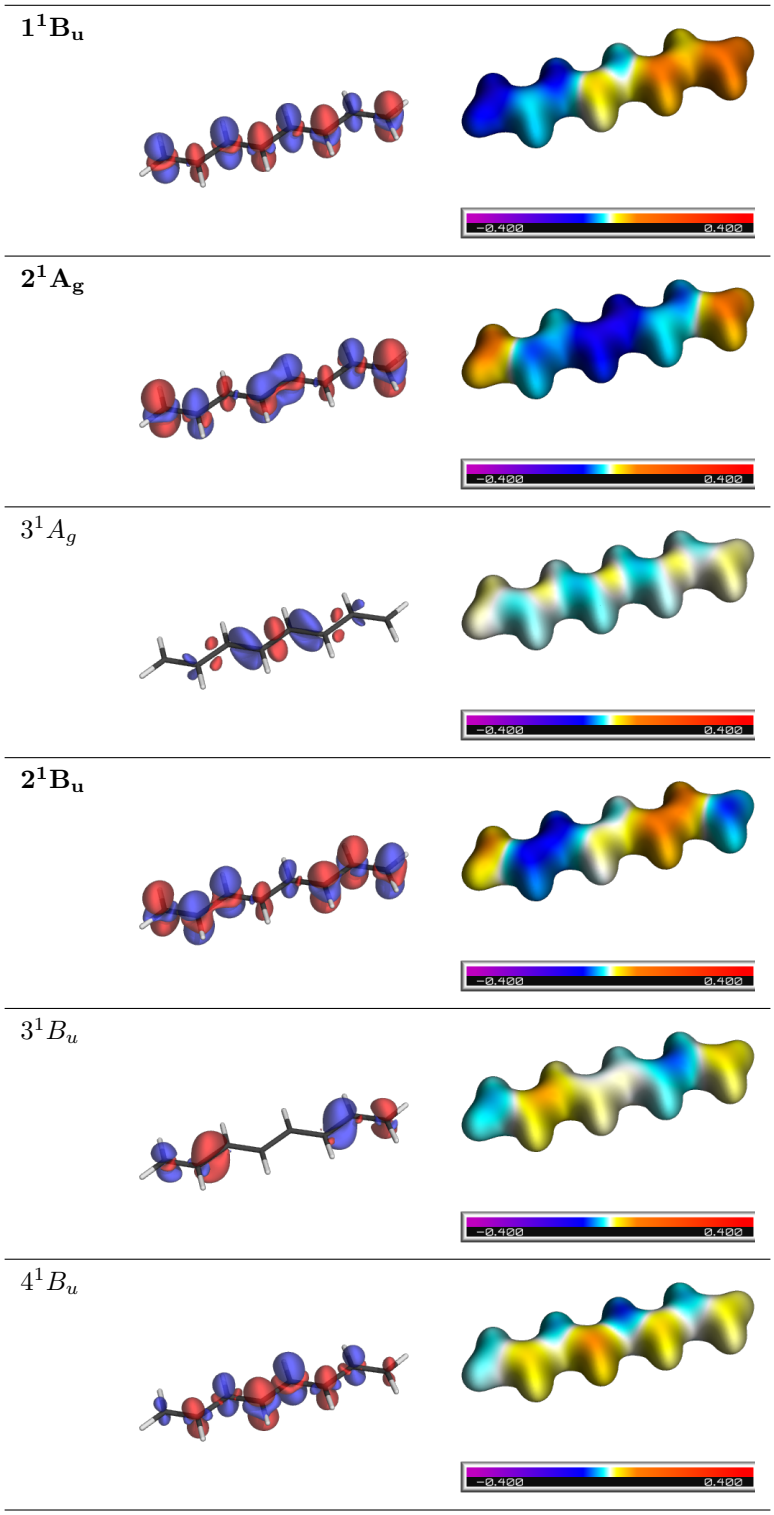


Figure S4 - transition densities and electrostatic potential maps of the $\pi\pi^*$ states of octatetraene computed at the CIS/aug-cc-PVTZ level of theory.