

Supporting Information for
“Investigation of Multiconfigurational
short-range Density Functional Theory for
Electronic Excitations in Organic Molecules”

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Table SI-1: Linear response excitation energies in eV, with oscillator strengths in parenthesis for allowed transitions. For CAS-srPBE(GWS) and HF-srPBE(GWS) the range separation parameter used is $\mu = 0.4$. The complete active spaces (CAS)ⁿ with n electron are specified for CAS-srPBE and CASSCF models, but not CASPT2. All basis sets are TZVP.

Molecule	State	CAS-srPBE(GWS)	HF	CASSCF	PBE	HF-srPBE(GWS)	CASPT2 ^a
<i>E</i> -Butadiene	$1^1B_u(\pi \rightarrow \pi^*)$	6.10 (0.731)	6.08 (0.893)	7.39 (0.813)	5.62 (0.609)	6.07 (0.750)	6.47 (0.783)
CAS: $(2a_u 2b_g)^4$	$2^1A_g(\pi \rightarrow \pi^*)$	6.94	8.02	6.97	6.30	8.00	6.62
all- <i>E</i> -Hexatriene	$1^1B_u(\pi \rightarrow \pi^*)$	5.09 (1.128)	5.16 (1.372)	6.58 (1.257)	4.52 (0.977)	5.11 (1.162)	5.31 (1.045)
CAS: $(1a_g 1b_u 3a_u 3b_g)^8$	$2^1A_g(\pi \rightarrow \pi^*)$	5.73	7.27	6.18	5.06	7.21	5.42
all- <i>E</i> -Octatetraene	$2^1A_g(\pi \rightarrow \pi^*)$	4.87	6.52	5.09	4.19	6.39	4.64
CAS: $(4a_u 4b_g)^8$	$1^1B_u(\pi \rightarrow \pi^*)$	4.43 (1.489)	4.55 (1.866)	6.04 (1.629)	3.83 (1.362)	4.49 (1.593)	4.70 (1.299)
Cyclopentadiene	$1^1B_2(\pi \rightarrow \pi^*)$	5.40 (0.096)	5.20 (0.096)	6.61 (0.085)	4.94 (0.087)	5.30 (0.095)	5.51 (0.144)
CAS: $(2b_1 2a_2)^4$	$2^1A_1(\pi \rightarrow \pi^*)$	6.75 (0.009)	8.37 (0.068)	6.87 (0.000)	6.09 (0.006)	7.40 (0.026)	6.31 (0.001)
	$3^1A_1(\pi \rightarrow \pi^*)$	8.35 (0.576)	8.38 (0.697)	9.26 (0.678)	8.06 (0.494)	8.34 (0.604)	8.52 (0.965)
Benzene	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.87	5.91	6.95	5.25	5.53	5.04
CAS: $(1b_{1u} 1b_{2g} 1b_{3g} 1a_u)^4$	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.57	5.93	7.08	6.03	6.28	6.42
	$1^1E_{1u}(\pi \rightarrow \pi^*)$	7.28 (0.627)	7.55 (0.724)	7.96 (0.711)	6.98 (0.556)	7.27 (0.629)	7.13 (0.847)
	$2^1E_{2g}(\pi \rightarrow \pi^*)$	9.20	10.39	9.02	8.29	9.91	8.18
Pyrazine	$1^1B_{3u}(n \rightarrow \pi^*)$	4.18 (0.007)	4.94 (0.008)	4.69 (0.012)	3.56 (0.004)	4.33 (0.007)	4.12 (0.012)
CAS ^b	$1^1A_u(n \rightarrow \pi^*)$	5.07	6.95	7.45	4.03	5.25	4.70
	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.69 (0.127)	5.66 (0.155)	4.55 (0.042)	5.26 (0.072)	5.38 (0.106)	4.85 (0.123)
	$1^1B_{2g}(n \rightarrow \pi^*)$	5.83	6.49	5.77	5.09	5.98	5.68
	$1^1B_{1g}(n \rightarrow \pi^*)$	6.93	9.05	9.66	5.54	7.18	6.41
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.96 (0.098)	6.28 (0.032)	7.75 (0.077)	6.44 (0.053)	6.68 (0.072)	6.89 (0.107)
	$2^1B_{1u}(\pi \rightarrow \pi^*)$	7.94 (0.391)	8.12 (0.564)	8.87 (0.478)	7.52 (0.241)	7.95 (0.437)	7.79 (0.774)
	$2^1B_{2u}(\pi \rightarrow \pi^*)^c$	8.07 (0.311)	8.64 (0.430)	8.76 (0.478)	7.69 (0.504)	8.06 (0.375)	7.66 (0.622)
	$1^1B_{3g}(\pi \rightarrow \pi^*)^d$	9.72	11.12	8.25	8.83	10.66	8.47
	$2^1A_g(\pi \rightarrow \pi^*)$	8.92	10.36	8.24	7.05	9.07	8.61
Formaldehyde	$1^1A_2(n \rightarrow \pi^*)$	3.81	4.28	4.34	3.77	3.86	3.99
CAS: $(2a_1, 2b_1, 2b_2)^6$	$1^1B_1(\sigma \rightarrow \pi^*)$	8.56 (0.082)	10.15 (0.110)	8.86 (0.053)	7.33 (0.086)	8.75 (0.075)	9.14 (0.013)
	$2^1A_1(\pi \rightarrow \pi^*)^e$	10.57 (0.320)	12.18 (0.271)	10.95(0.336)	9.94 (0.316)	10.74(0.297)	9.32 (0.451)
Acetone	$1^1A_2(n \rightarrow \pi^*)$	4.31	4.93	4.45	4.20	4.39	4.44
CAS: $(1a_1, 1b_1, 2b_2)^2$	$1^1B_1(\sigma \rightarrow \pi^*)^f$	8.11 (0.029)	11.43 (0.054)	9.67 (0.045)	7.68 (0.029)	9.81 (0.026)	9.27 (0.011)
	$2^1A_1(\pi \rightarrow \pi^*)^g$	9.12 (0.214)	9.26 (0.286)	9.15 (0.302)	8.69 (0.269)	9.13 (0.209)	9.31 (0.358)
Acetamide	$1^1A''(n \rightarrow \pi^*)$	5.59 (0.001)	6.42 (0.001)	6.18 (0.000)	5.40 (0.001)	5.64 (0.001)	5.69 (0.001)
CAS ^h	$2^1A'(\pi \rightarrow \pi^*)$	7.64 (0.109)	8.72 (0.232)	8.62 (0.267)	5.68 (0.027)	7.85 (0.132)	7.27 (0.424)
	$3^1A'(\pi \rightarrow \pi^*)$	8.12 (0.143)	9.84 (0.085)	8.86 (0.085)	6.88 (0.010)	8.27 (0.123)	10.09(0.263)

^a See Ref. 1

^b CAS($2a_g, 1b_{3u}, 1b_{2u}, 1b_{1g}, 1b_{1u}, 1b_{2g}, 1b_{3g}, 1a_u$)⁶ for CAS-srPBE(GWS) and CAS($2b_{3u}, 1b_{1g}, 2b_{2g}, 1a_u$)⁶ for CASSCF

^c This pyrazine state corresponds to 3^1B_{2u} for PBE.

^d This pyrazine state corresponds to 2^1B_{3g} for PBE.

^e This formaldehyde state corresponds to 4^1A_1 for CAS-srPBE(GWS), 3^1A_1 for HF, CASSCF, PBE and HF-srPBE(GWS).

^f This acetone state corresponds to 2^1B_1 for HF, PBE and HF-srPBE(GWS).

^g This acetone state corresponds to 4^1A_1 for PBE.

^h CAS($3a', 2a''$)⁴ for CAS-srPBE(GWS) and CAS($4a', 2a''$)⁶ for CASSCF.

Table SI-1 (Continued.)

Molecule	State	CAS-srPBE(GWS)	HF	CASSCF	PBE	HF-srPBE(GWS)	CASPT2 ^a
Cytosine CAS(8a', 6a'') ¹²	2 ¹ A'(π → π*)	4.95 (0.062)	5.82 (0.140)	5.53 (0.080)	4.20 (0.015)	5.16 (0.080)	4.67 (0.093)
	1 ¹ A''(n → π*)	5.23 (0.002)	6.74 (0.002)	5.70 (0.000)	3.78 (0.000)	5.45 (0.002)	5.12 (0.003)
	2 ¹ A''(n → π*)	5.88 (0.000)	7.06 (0.000)	6.18 (0.004)	4.47 (0.001)	6.00 (0.000)	5.53 (0.002)
	3 ¹ A'(π → π*)	5.90 (0.127)	7.21 (0.355)	7.01 (0.486)	4.91 (0.059)	6.24 (0.210)	5.53 (0.352)
	4 ¹ A'(π → π*)	6.67 (0.484)	7.72 (0.500)	7.35 (0.419)	5.62 (0.010)	6.91 (0.503)	6.40 (0.623)
	5 ¹ A'(π → π*)	7.09 (0.228)	8.91 (0.162)	8.69 (0.037)	5.95 (0.023)	7.40 (0.171)	6.97 (0.366)
Thymine CAS(6a', 6a'') ¹²	6 ¹ A'(π → π*)	8.08 (0.021)	9.98 (0.140)	9.67 (0.251)	6.02 (0.066)	8.44 (0.035)	8.23 (0.132)
	1 ¹ A''(n → π*)	4.98 (0.000)	6.06 (0.000)	5.03 (0.000)	4.07 (0.000)	5.19 (0.000)	4.95 (0.000)
	2 ¹ A'(π → π*)	5.36 (0.193)	6.00 (0.369)	6.46 (0.399)	4.59 (0.071)	5.43 (0.229)	5.06 (0.334)
	3 ¹ A'(π → π*)	6.64 (0.079)	8.01 (0.142)	7.62 (0.069)	5.32 (0.062)	6.98 (0.116)	6.15 (0.067)
	2 ¹ A''(n → π*)	6.44 (0.000)	7.51 (0.000)	6.61 (0.000)	4.78 (0.000)	6.48 (0.000)	6.38 (0.000)
	4 ¹ A'(π → π*)	6.66 (0.192)	8.45 (0.394)	8.34 (0.419)	5.83 (0.079)	7.11 (0.247)	6.53 (0.356)
	3 ¹ A''(n → π*)	7.28 (0.000)	7.58 (0.001)	7.56 (0.000)	5.32 (0.000)	7.28 (0.000)	6.85 (0.000)
	4 ¹ A''(n → π*)	7.30 (0.000)	8.56 (0.003)	8.76 (0.000)	5.86 (0.000)	7.88 (0.001)	7.43 (0.000)
Uracil CAS(6a', 6a'') ¹²	5 ¹ A''(n → π*)	7.47 (0.000)	8.86 (0.000)	8.97 (0.001)	6.12 (0.000)	8.00 (0.000)	-
	5 ¹ A'(π → π*)	7.61 (0.439)	9.40 (0.119)	9.07 (0.161)	6.04 (0.053)	8.04 (0.327)	7.43 (0.672)
	1 ¹ A''(n → π*)	4.93 (0.000)	6.06 (0.000)	6.07 (0.000)	3.65 (0.000)	5.16 (0.000)	4.91 (0.000)
	2 ¹ A'(π → π*) ^b	5.52 (0.199)	6.18 (0.379)	7.43 (0.340)	4.76 (0.056)	5.61 (0.225)	5.23 (0.320)
	3 ¹ A'(π → π*) ^c	6.60 (0.056)	8.12 (0.115)	6.71 (0.250)	5.20 (0.045)	7.02 (0.068)	6.15 (0.047)
	2 ¹ A''(n → π*)	6.38 (0.000)	7.45 (0.000)	6.50 (0.000)	4.74 (0.000)	6.42 (0.000)	6.28 (0.000)
	3 ¹ A''(n → π*)	7.20 (0.000)	7.79 (0.002)	7.80 (0.000)	5.22 (0.000)	7.49 (0.000)	6.98 (0.000)
	4 ¹ A'(π → π*)	6.83 (0.146)	8.58 (0.378)	8.37 (0.387)	5.88 (0.013)	7.23 (0.218)	6.74 (0.249)
Adenine CAS(4a', 8a'') ¹²	4 ¹ A''(n → π*)	7.46 (0.001)	8.90 (0.000)	8.99 (0.000)	6.08 (0.000)	7.82 (0.001)	7.28 (0.000)
	5 ¹ A''(n → π*)	7.50 (0.000)	9.30 (0.037)	9.27 (0.000)	6.10 (0.000)	7.93 (0.000)	-
	5 ¹ A'(π → π*) ^d	7.63 (0.466)	9.29 (0.179)	10.67 (0.187)	6.12 (0.109)	7.95 (0.389)	7.43 (0.804)
	2 ¹ A'(π → π*) ^e	5.47 (0.266)	6.16 (0.028)	5.09 (0.002)	5.00 (0.049)	5.55 (0.248)	5.20 (0.146)
	3 ¹ A'(π → π*) ^f	5.54 (0.027)	5.94 (0.346)	6.13 (0.258)	4.57 (0.120)	5.59 (0.083)	5.29 (0.201)
Adenine CAS(4a', 8a'') ¹²	1 ¹ A''(n → π*)	5.48 (0.001)	6.92 (0.000)	6.27 (0.008)	4.28 (0.000)	5.56 (0.000)	5.19 (0.001)
	2 ¹ A''(n → π*)	6.03 (0.002)	7.34 (0.001)	6.62 (0.003)	5.03 (0.001)	6.18 (0.002)	5.96 (0.002)
	4 ¹ A'(π → π*) ^g	6.36 (0.037)	7.83 (0.416)	7.26 (0.459)	5.56 (0.053)	6.85 (0.499)	6.34 (0.538)
	5 ¹ A'(π → π*) ^h	6.74 (0.480)	7.39 (0.183)	6.88 (0.104)	5.83 (0.093)	7.26 (0.027)	6.64 (0.001)
	6 ¹ A'(π → π*)	7.14 (0.072)	8.04 (0.427)	7.82 (0.009)	6.01 (0.021)	7.31 (0.184)	6.87 (0.010)
	7 ¹ A'(π → π*)	7.37 (0.190)	8.72 (0.087)	8.15 (0.407)	6.24 (0.073)	7.81 (0.146)	7.56 (0.037)

^a See Ref. 1^b This uracil state corresponds to 3¹A' for CASSCF.^c This uracil state corresponds to 2¹A' for CASSCF.^d This uracil state corresponds to 6¹A' for CASSCF.^e This adenine state corresponds to 3¹A' for HF and PBE.^f This adenine state corresponds to 2¹A' for HF and PBE.^g This adenine state corresponds to 5¹A' for HF and CASSCF.^h This adenine state corresponds to 4¹A' for HF and CASSCF.

Table SI-2: Comparison of Ahlrichs TZVP, Dunning cc-pVTZ and aug-cc-pVTZ basis sets for the CAS-srPBE(GWS) model. Linear response excitation energies in eV, with oscillator strengths for allowed transitions in parenthesis. For CAS-srPBE(GWS) the range separation parameter was $\mu = 0.4$. Δ_{TZ} and Δ_{aTZ} are respectively the change for cc-pVTZ and aug-cc-pVTZ relative to TZVP, significant basis effects (> 0.4 eV) are marked in bold face. The listed CAS spaces are for CAS-srPBE(GWS), not CASPT2.

Molecule	State	CAS-srPBE(GWS) $\mu = 0.4$			Basis effects		CASPT2 ^a	
		TZVP	cc-pVTZ	aug-cc-pVTZ	Δ_{TZ}	Δ_{aTZ}	TZVP	aug-cc-pVTZ
<i>E</i> -Butadiene CAS(2 <i>a_u</i> , 2 <i>b_g</i>) ⁴	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	6.10 (0.731)	6.10 (0.714)	5.93 (0.695)	0.00	-0.17	6.47 (0.783)	6.38 (0.635)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	6.94	6.98	6.81	0.04	-0.13	6.62	6.43
all- <i>E</i> -Hexatriene CAS(1 <i>a_g</i> , 1 <i>b_u</i> , 3 <i>a_u</i> , 3 <i>b_g</i>) ⁸	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	5.09 (1.128)	5.07 (1.111)	4.98 (1.114)	-0.02	-0.11	5.31 (1.045)	5.18 (0.981)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	5.73	5.75	5.71	0.02	-0.02	5.42	5.33
all- <i>E</i> -Octatetraene CAS(4 <i>a_u</i> , 4 <i>b_g</i>) ⁸	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	4.87	4.88	4.86	0.01	-0.01	4.64	4.52
	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	4.43 (1.489)	4.41 (1.530)	4.35 (1.541)	-0.02	-0.08	4.70 (1.299)	4.35 (1.307)
Cyclopentadiene CAS(2 <i>b₁</i> , 2 <i>a₂</i>) ⁴	1 ¹ <i>B₂</i> ($\pi \rightarrow \pi^*$)	5.40 (0.096)	5.36 (0.088)	5.30 (0.089)	-0.04	-0.10	5.51 (0.144)	5.43 (0.117)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	6.75 (0.009)	6.73 (0.009)	6.65 (0.003)	-0.02	-0.10	6.31 (0.001)	6.28 (0.000)
	3 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	8.35 (0.576)	8.34 (0.527)	8.03 (0.407)	-0.01	-0.32	8.52 (0.965)	8.15 (0.642)
Benzene CAS(1 <i>b_{1u}</i> , 1 <i>b_{2g}</i> , 1 <i>b_{3g}</i> , 1 <i>a_u</i>) ⁴	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.87	5.87	5.82	0.00	-0.05	5.04	4.96
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.57	6.55	6.48	-0.02	-0.09	6.42	6.57
	1 ¹ <i>E_{1u}</i> ($\pi \rightarrow \pi^*$)	7.28 (0.627)	7.27 (0.605)	7.13 (0.624)	-0.01	-0.15	7.13 (0.847)	7.36 (0.787)
	2 ¹ <i>E_{2g}</i> ($\pi \rightarrow \pi^*$)	9.20	9.13	8.98	-0.07	-0.22	8.18	8.15
Pyrazine CAS ^b	1 ¹ <i>B_{3u}</i> ($n \rightarrow \pi^*$)	4.18 (0.007)	4.17 (0.005)	4.15 (0.006)	-0.01	-0.03	4.12 (0.012)	4.02 (0.009)
	1 ¹ <i>A_u</i> ($n \rightarrow \pi^*$)	5.07	5.05	5.06	-0.02	-0.01	4.70	4.75
	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.69 (0.127)	5.67 (0.127)	5.61 (0.137)	-0.02	-0.08	4.85 (0.123)	4.80 (0.127)
	1 ¹ <i>B_{2g}</i> ($n \rightarrow \pi^*$)	5.83	5.82	5.80	-0.01	-0.03	5.68	5.56
	1 ¹ <i>B_{1g}</i> ($n \rightarrow \pi^*$)	6.93	6.93	6.93	0.00	0.00	6.41	6.47
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.96 (0.098)	6.91 (0.099)	6.86 (0.085)	-0.05	-0.10	6.89 (0.107)	6.61 (0.176)
	2 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	7.94 (0.391)	7.91 (0.348)	7.71 (0.418)	-0.03	-0.23	7.79 (0.774)	7.71 (0.620)
	2 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$) ^c	8.07 (0.311)	8.07 (0.298)	7.99 (0.279)	0.00	-0.08	7.66 (0.622)	7.73 (0.598)
	1 ¹ <i>B_{3g}</i> ($\pi \rightarrow \pi^*$) ^d	9.72	9.65	9.47	-0.07	-0.25	8.47	8.33
2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$) ^e	8.92	8.84	8.63	-0.08	-0.29	8.61	8.30	
Formaldehyde CAS(2 <i>a₁</i> , 2 <i>b₁</i> , 2 <i>b₂</i>) ⁶	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	3.81	3.83	3.80	0.02	-0.01	3.99	4.01
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.56 (0.082)	8.33 (0.090)	7.21 (0.017)	-0.23	-1.35	9.14 (0.013)	9.12 (0.012)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^f	10.57 (0.320)	10.41 (0.344)	9.35 (0.137)	-0.16	-1.22	9.32 (0.451)	9.47 (0.242)
Acetone CAS(1 <i>a₁</i> , 1 <i>b₁</i> , 2 <i>b₂</i>) ²	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	4.31	4.33	4.31	0.02	0.00	4.44	4.49
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.11 (0.029)	8.16 (0.032)	7.00 (0.030)	0.05	-1.11	9.27 (0.011)	9.25 (0.009)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^g	9.12 (0.214)	9.08 (0.186)	8.99 (0.264)	-0.04	-0.13	9.31 (0.358)	9.19 (0.357)
Acetamide CAS(3 <i>a'</i> , 2 <i>a''</i>) ⁴	1 ¹ <i>A''</i> ($n \rightarrow \pi^*$)	5.59 (0.001)	5.62 (0.001)	5.53 (0.000)	0.03	-0.06	5.69 (0.001)	5.69 (0.002)
	2 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.64 (0.109)	7.70 (0.095)	6.96 (0.024)	0.06	-0.68	7.27 (0.424)	7.12 (0.299)
	3 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	8.12 (0.143)	8.16 (0.135)	7.39 (0.186)	0.04	-0.73	10.09 (0.263)	10.03(0.164)

^a See reference 1

^b CAS(2*a_g*, 1*b_{3u}*, 1*b_{2u}*, 1*b_{1g}*, 1*b_{1u}*, 1*b_{2g}*, 1*b_{3g}*, 1*a_u*)⁶ for CAS-srPBE(GWS).

^c This pyrazine state corresponds to 3¹*B_{2u}* for CAS-srPBE(GWS) in aug-cc-pVTZ.

^d This pyrazine state corresponds to 2¹*B_{3g}* for CAS-srPBE(GWS) in aug-cc-pVTZ.

^e This pyrazine state corresponds to 3¹*A_g* for CAS-srPBE(GWS) in aug-cc-pVTZ.

^f This formaldehyde state corresponds to 4¹*A₁* for CAS-srPBE(GWS) in the three basis sets.

^g This acetone state corresponds to 4¹*A₁* for CAS-srPBE(GWS) in aug-cc-pVTZ.

Table SI-2 (Continued.)

Molecule	State	CAS-srPBE(GWS) $\mu = 0.4$			Basis effects		CASPT2 ^a	
		TZVP	cc-pVTZ	aug-cc-pVTZ	Δ_{TZ}	Δ_{aTZ}	TZVP	aug-cc-pVTZ
Cytosine CAS(4a', 6a'') ¹⁰	2 ¹ A'($\pi \rightarrow \pi^*$)	4.93 (0.061)	4.93 (0.058)	4.87 (0.060)	0.00	-0.06	4.67 (0.093)	4.52 (0.053)
	1 ¹ A''($n \rightarrow \pi^*$)	5.06 (0.002)	5.08 (0.001)	5.05 (0.002)	0.02	-0.01	5.12 (0.003)	5.03 (0.003)
	2 ¹ A''($n \rightarrow \pi^*$)	5.83 (0.000)	5.90 (0.000)	5.85 (0.000)	0.07	0.02	5.53 (0.002)	5.44 (0.001)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.95 (0.128)	5.95 (0.126)	5.84 (0.136)	0.00	-0.11	5.53 (0.352)	5.43 (0.238)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.62 (0.460)	6.49 (0.341)	6.18 (0.311)	-0.13	-0.44	6.40 (0.623)	6.09 (0.546)
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.10 (0.273)	7.14 (0.221)	6.86 (0.108)	0.04	-0.24	6.97 (0.366)	6.68 (0.406)
	6 ¹ A'($\pi \rightarrow \pi^*$)	8.35 (0.067)	7.61 (0.126)	7.18 (0.271)	-0.74	-1.17	8.23 (0.132)	-
Thymine CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.98 (0.000)	5.12 (0.000)	4.98 (0.000)	0.14	0.00	4.95 (0.000)	4.86 (-)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.36 (0.193)	5.23 (0.164)	5.18 (0.095)	-0.13	-0.18	5.06 (0.334)	4.91 (0.278)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.64 (0.079)	6.63 (0.060)	5.63 (0.201)	-0.01	-1.01	6.15 (0.067)	6.01 (0.067)
	2 ¹ A''($n \rightarrow \pi^*$)	6.44 (0.000)	6.39 (0.000)	6.38 (0.000)	-0.05	-0.06	6.38 (0.000)	6.22 (-)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.66 (0.192)	6.73 (0.218)	6.54 (0.212)	0.07	-0.12	6.53 (0.356)	6.32 (0.283)
	3 ¹ A''($n \rightarrow \pi^*$)	7.28 (0.000)	7.22 (0.000)	6.40 (0.000)	-0.06	-0.88	6.85 (0.000)	6.59 (-)
	4 ¹ A''($n \rightarrow \pi^*$)	7.30 (0.000)	7.29 (0.000)	7.13 (0.001)	-0.01	-0.17	7.43 (0.000)	7.05 (-)
	5 ¹ A''($n \rightarrow \pi^*$)	7.47 (0.000)	7.46 (0.000)	7.31 (0.001)	-0.01	-0.16	-	-
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.61 (0.439)	7.82 (0.401)	6.70 (0.006)	0.21	-0.91	7.43 (0.672)	7.33 (0.680)
Uracil CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.93 (0.000)	4.95 (0.000)	4.94 (0.000)	0.02	0.01	4.91 (0.000)	4.80
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.52 (0.199)	5.47 (0.166)	5.38 (0.157)	-0.00	-0.14	5.23 (0.320)	5.06 (0.276)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.60 (0.056)	6.55 (0.078)	6.36 (0.175)	-0.00	-0.24	6.15 (0.047)	6.00 (0.045)
	2 ¹ A''($n \rightarrow \pi^*$)	6.38 (0.000)	6.39 (0.000)	6.32 (0.000)	0.01	-0.06	6.28 (0.000)	6.15
	3 ¹ A''($n \rightarrow \pi^*$)	7.20 (0.000)	7.23 (0.000)	6.63 (0.004)	0.03	-0.57	6.98 (0.000)	6.73
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.83 (0.146)	6.78 (0.142)	6.58 (0.099)	-0.05	-0.25	6.74 (0.249)	6.47 (0.259)
	4 ¹ A''($n \rightarrow \pi^*$)	7.46 (0.001)	7.42 (0.001)	7.17 (0.001)	-0.04	-0.29	7.28 (0.000)	6.93
	5 ¹ A''($n \rightarrow \pi^*$)	7.50 (0.000)	7.47 (0.000)	7.41 (0.000)	-0.03	-0.09	-	-
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.63 (0.466)	7.27 (0.283)	6.90 (0.191)	-0.36	-0.73	7.43 (0.804)	7.37 (0.212)
	Adenine CAS(4a', 8a'') ¹²	2 ¹ A'($\pi \rightarrow \pi^*$)	5.47 (0.266)	5.42 (0.226)	5.31 (0.235)	-0.05	-0.16	5.20 (0.146)
3 ¹ A'($\pi \rightarrow \pi^*$)		5.54 (0.027)	5.52 (0.047)	5.48 (0.043)	-0.02	-0.06	5.29 (0.201)	5.02 (0.015)
1 ¹ A''($n \rightarrow \pi^*$)		5.48 (0.001)	5.46 (0.000)	5.44 (0.001)	-0.02	-0.04	5.19 (0.001)	5.04 (0.002)
2 ¹ A''($n \rightarrow \pi^*$)		6.03 (0.002)	6.03 (0.002)	5.98 (0.002)	0.00	-0.05	5.96 (0.002)	5.75 (0.007)
4 ¹ A'($\pi \rightarrow \pi^*$)		6.36 (0.037)	6.21 (0.032)	6.10 (0.045)	-0.15	-0.26	6.34 (0.538)	6.25 (0.510)
5 ¹ A'($\pi \rightarrow \pi^*$)		6.74 (0.480)	6.72 (0.447)	6.59 (0.470)	-0.02	-0.15	6.64 (0.001)	6.65 (0.069)
6 ¹ A'($\pi \rightarrow \pi^*$)		7.14 (0.072)	7.12 (0.063)	6.96 (0.032)	-0.02	-0.18	6.87 (0.010)	6.96 (0.344)
7 ¹ A'($\pi \rightarrow \pi^*$)		7.37 (0.190)	7.33 (0.181)	7.18 (0.208)	-0.04	-0.19	7.56 (0.037)	7.55 (0.036)

^aSee reference 1

Table SI-3: CAS-srPBE(GWS): Dependency of excitation energies (in eV) and oscillator strengths on the range separation parameter μ . Calculated oscillator strengths for allowed transitions are given in parenthesis after the excitation energy.

Molecule	State μ parameter	CAS-srPBE(GWS)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
<i>E</i> -Butadiene CAS(2 <i>a_u</i> , 2 <i>b_g</i>) ⁴	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$) ^a	5.99 (0.705)	6.10 (0.731)	6.26 (0.759)	6.60 (0.798)	6.84 (0.812)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	6.89	6.94	6.99	7.04	7.05
all- <i>E</i> -Hexatriene CAS(1 <i>a_g</i> , 1 <i>b_u</i> , 3 <i>a_u</i> , 3 <i>b_g</i>) ⁸	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	4.96 (1.094)	5.09 (1.128)	5.29 (1.166)	5.69 (1.223)	5.95 (1.245)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	5.67	5.73	5.83	5.97	6.06
all- <i>E</i> -Octatetraene CAS(4 <i>a_u</i> , 4 <i>b_g</i>) ⁸	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	4.83	4.87	4.92	5.01	5.05
	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	4.31 (1.508)	4.43 (1.489)	4.64 (1.590)	5.07 (1.654)	5.36 (1.676)
Cyclopentadiene CAS(2 <i>b₁</i> , 2 <i>a₂</i>) ⁴	1 ¹ <i>B₂</i> ($\pi \rightarrow \pi^*$) ^b	5.30 (0.095)	5.40 (0.096)	5.53 (0.096)	5.83 (0.094)	6.04 (0.092)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	6.66 (0.010)	6.75 (0.009)	6.83 (0.007)	6.92 (0.003)	6.94 (0.002)
	3 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	8.23 (0.461)	8.35 (0.576)	8.48 (0.632)	8.72 (0.667)	8.89 (0.677)
Benzene CAS(1 <i>b_{1u}</i> , 1 <i>b_{2g}</i> , 1 <i>b_{3g}</i> , 1 <i>a_u</i>) ⁴	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.70	5.87	6.09	6.23	6.63
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.49	6.57	6.64	6.72	6.78
	1 ¹ <i>E_{1u}</i> ($\pi \rightarrow \pi^*$)	7.20 (0.612)	7.28 (0.627)	7.39 (0.646)	7.58 (0.679)	7.68 (0.692)
	2 ¹ <i>E_{2g}</i> ($\pi \rightarrow \pi^*$)	9.11	9.20	9.27	9.26	9.20
Pyrazine CAS ^c	1 ¹ <i>B_{3u}</i> ($n \rightarrow \pi^*$)	4.13 (0.007)	4.26 (0.007)	4.40 (0.008)	4.58 (0.008)	4.69 (0.016)
	1 ¹ <i>A_u</i> ($n \rightarrow \pi^*$)	4.89	5.17	5.55	6.30	6.79
	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.37 (0.094)	5.37 (0.097)	5.33 (0.097)	5.14 (0.085)	4.98 (0.073)
	1 ¹ <i>B_{2g}</i> ($n \rightarrow \pi^*$)	5.68	5.77	5.86	5.92	5.91
	1 ¹ <i>B_{1g}</i> ($n \rightarrow \pi^*$)	6.60	6.97	7.47	8.53	9.21
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.75 (0.078)	6.81 (0.077)	6.86 (0.072)	6.95 (0.060)	7.05 (0.056)
	2 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	7.86 (0.409)	7.93 (0.428)	8.01 (0.452)	8.17 (0.490)	8.32 (0.503)
	2 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	7.90 (0.367)	7.98 (0.382)	8.08 (0.401)	8.25 (0.438)	8.36 (0.459)
	1 ¹ <i>B_{3g}</i> ($\pi \rightarrow \pi^*$)	9.31	9.31	9.26	9.03	8.83
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	8.64	8.97	8.96	8.77	8.64
Formaldehyde CAS(2 <i>a₁</i> , 2 <i>b₁</i> , 2 <i>b₂</i>) ⁶	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	3.78	3.81	3.87	4.01	4.11
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.29 (0.080)	8.56 (0.082)	8.85 (0.085)	9.11 (0.088)	9.16 (0.088)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^d	10.37 (0.337)	10.57(0.320)	10.81 (0.307)	11.05 (0.303)	11.11 (0.305)
Acetone CAS(1 <i>a₁</i> , 1 <i>b₁</i> , 2 <i>b₂</i>) ²	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	4.28	4.31	4.35	4.39	4.39
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	7.66 (0.028)	8.11 (0.029)	8.62 (0.031)	9.38 (0.034)	9.71 (0.037)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	8.95 (0.165)	9.12 (0.214)	9.23 (0.251)	9.25 (0.284)	9.18 (0.295)
Acetamide CAS(3 <i>a'</i> , 2 <i>a''</i>) ⁴	1 ¹ <i>A''</i> ($n \rightarrow \pi^*$)	5.54 (0.001)	5.59 (0.001)	5.65 (0.001)	5.81 (0.001)	5.93 (0.001)
	2 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.38 (0.030)	7.64 (0.109)	7.92 (0.142)	8.38 (0.189)	8.58 (0.201)
	3 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.81 (0.192)	8.12 (0.143)	8.50 (0.114)	9.05 (0.088)	9.20 (0.087)

^a For butadiene CAS-srPBE(GWS) with $\mu \in \{0.33, 0.5, 0.75, 1\}$, a triplet 1³*B_u* comes before the 1¹*B_u* state in the response function.

^b For cyclopentadiene CAS-srPBE(GWS) with $\mu = 0.4$, a triplet 1³*B₂* comes before the 1¹*B₂* state in the response function.
^c CAS(2*a_g*, 1*b_{3u}*, 1*b_{2u}*, 1*b_{1g}*, 1*b_{1u}*, 1*b_{2g}*, 1*b_{3g}*, 1*a_u*)⁶ for CAS-srPBE(GWS).

^d This formaldehyde state corresponds to 4¹*A₁* for CAS-srPBE(GWS) with $\mu \in \{0.33, 0.4, 0.5\}$, 3¹*A₁* for CAS-srPBE(GWS) with $\mu \in \{0.75, 1\}$.

Table SI-3 (Continued.)

Molecule	State μ parameter	CAS-srPBE(GWS)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
Cytosine CAS(8a', 6a'') ¹²	2 ¹ A'($\pi \rightarrow \pi^*$)	4.84 (0.053)	4.95 (0.062)	5.10 (0.079)	5.23 (0.105)	5.24 (0.115)
	1 ¹ A''($n \rightarrow \pi^*$)	5.07 (0.002)	5.23 (0.002)	5.39 (0.002)	5.62 (0.002)	5.74 (0.002)
	2 ¹ A''($n \rightarrow \pi^*$)	5.64 (0.000)	5.88 (0.000)	6.12 (0.000)	6.55 (0.000)	6.82 (0.000)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.73 (0.119)	5.90 (0.127)	6.11 (0.110)	6.41 (0.088)	6.52 (0.067)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.62 (0.363)	6.67 (0.484)	6.87 (0.560)	7.11 (0.639)	7.23 (0.676)
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.76 (0.167)	7.09 (0.228)	7.37 (0.220)	7.90 (0.191)	8.18 (0.180)
	6 ¹ A'($\pi \rightarrow \pi^*$)	6.98 (0.197)	8.08 (0.021)	8.68 (0.152)	9.09 (0.180)	9.24 (0.178)
Thymine CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.88 (0.000)	4.98 (0.000)	5.30 (0.000)	5.14 (0.000)	5.18 (0.000)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.16 (0.162)	5.36 (0.193)	5.41 (0.181)	6.04 (0.295)	6.30 (0.335)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.84 (0.049)	6.64 (0.079)	6.84 (0.144)	7.65 (0.120)	7.91 (0.105)
	2 ¹ A''($n \rightarrow \pi^*$)	6.23 (0.000)	6.44 (0.000)	6.48 (0.000)	6.37 (0.000)	6.40 (0.000)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.50 (0.041)	6.66 (0.192)	7.01 (0.268)	7.75 (0.318)	8.09 (0.391)
	3 ¹ A''($n \rightarrow \pi^*$)	6.90 (0.000)	7.28 (0.000)	7.59 (0.000)	7.82 (0.000)	7.88 (0.000)
	4 ¹ A''($n \rightarrow \pi^*$)	6.97 (0.000)	7.30 (0.000)	7.79 (0.000)	8.94 (0.000)	9.04 (0.001)
	5 ¹ A''($n \rightarrow \pi^*$)	7.04 (0.000)	7.47 (0.000)	7.98 (0.000)	8.98 (0.007)	9.21 (0.002)
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.56 (0.171)	7.61 (0.439)	7.85 (0.357)	8.65 (0.264)	8.98 (0.183)
Uracil CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.81 (0.000)	4.93 (0.000)	5.27 (0.000)	5.12 (0.000)	5.16 (0.000)
	2 ¹ A'($\pi \rightarrow \pi^*$) ^a	5.33 (0.151)	5.52 (0.199)	5.58 (0.186)	6.17 (0.303)	6.40 (0.345)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.36 (0.048)	6.60 (0.056)	6.91 (0.059)	7.66 (0.109)	7.94 (0.112)
	2 ¹ A''($n \rightarrow \pi^*$)	6.14 (0.000)	6.38 (0.000)	6.42 (0.000)	6.33 (0.000)	6.37 (0.000)
	3 ¹ A''($n \rightarrow \pi^*$)	6.70 (0.000)	7.20 (0.000)	7.78 (0.001)	8.00 (0.001)	8.05 (0.001)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.71 (0.144)	6.83 (0.146)	7.07 (0.248)	7.92 (0.251)	8.25 (0.320)
	4 ¹ A''($n \rightarrow \pi^*$)	6.89 (0.000)	7.46 (0.001)	7.82 (0.000)	9.03 (0.006)	9.23 (0.000)
	5 ¹ A''($n \rightarrow \pi^*$)	7.24 (0.000)	7.50 (0.000)	7.85 (0.001)	9.17 (0.000)	9.34 (0.007)
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.55 (0.450)	7.63 (0.466)	7.78 (0.431)	8.56 (0.330)	8.89 (0.247)
Adenine CAS(4a', 8a'') ¹²	2 ¹ A'($\pi \rightarrow \pi^*$) ^b	5.43 (0.016)	5.54 (0.027)	5.61 (0.100)	5.59 (0.017)	5.46 (0.014)
	3 ¹ A'($\pi \rightarrow \pi^*$) ^b	5.33 (0.274)	5.47 (0.266)	5.66 (0.211)	5.92 (0.283)	5.90 (0.293)
	1 ¹ A''($n \rightarrow \pi^*$) ^c	5.23 (0.000)	5.48 (0.001)	5.74 (0.001)	6.52 (0.004)	6.25 (0.003)
	2 ¹ A''($n \rightarrow \pi^*$) ^c	5.84 (0.002)	6.03 (0.002)	6.24 (0.003)	6.13 (0.002)	6.64 (0.003)
	4 ¹ A'($\pi \rightarrow \pi^*$) ^d	6.57 (0.439)	6.74 (0.480)	6.88 (0.511)	7.10 (0.469)	7.22 (0.413)
	5 ¹ A'($\pi \rightarrow \pi^*$) ^d	6.70 (0.003)	6.36 (0.037)	7.07 (0.029)	7.27 (0.111)	6.94 (0.168)
	6 ¹ A'($\pi \rightarrow \pi^*$)	6.96 (0.094)	7.14 (0.072)	7.36 (0.109)	7.65 (0.145)	7.75 (0.082)
	7 ¹ A'($\pi \rightarrow \pi^*$)	7.40 (0.211)	7.37 (0.190)	7.66 (0.256)	7.90 (0.250)	7.96 (0.302)

^a For uracil CAS-srPBE(GWS) with $\mu = 0.33$, there is an intruder state before 2¹A' : 3.43 (0.018).

^b For adenine CAS-srPBE(GWS) with $\mu \in \{0.33, 0.4\}$, 2¹A' and 3¹A' correspond respectively to 3¹A' and 2¹A' in the response function.

^c For adenine CAS-srPBE(GWS) with $\mu = 0.75$, 1¹A'' and 2¹A'' correspond respectively to 2¹A'' and 1¹A'' in the response function.

^d For adenine CAS-srPBE(GWS) with $\mu \in \{0.4, 1\}$, 4¹A' and 5¹A' correspond respectively to 5¹A' and 4¹A' in the response function.

Table SI-4: HF-srPBE(GWS): μ dependency and oscillator strengths for allowed transitions in parenthesis.

Molecule	State μ parameter	HF-srPBE(GWS)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
<i>E</i> -Butadiene	$1^1B_u(\pi \rightarrow \pi^*)^a$	6.01 (0.720)	6.08 (0.750)	6.13 (0.785)	6.14 (0.839)	6.12 (0.864)
	$2^1A_g(\pi \rightarrow \pi^*)$	7.75	7.98	8.10	8.12	8.10
all- <i>E</i> -Hexatriene	$1^1B_u(\pi \rightarrow \pi^*)$	5.02 (1.122)	5.11 (1.161)	5.18 (1.209)	5.21 (1.287)	5.20 (1.326)
	$2^1A_g(\pi \rightarrow \pi^*)$	6.99	7.22	7.27	7.30	7.29
all- <i>E</i> -Octatetraene	$2^1A_g(\pi \rightarrow \pi^*)$	6.26	6.40	6.47	6.53	6.53
	$1^1B_u(\pi \rightarrow \pi^*)$	4.40 (1.544)	4.49 (1.591)	4.56 (1.651)	4.60 (1.751)	4.59 (1.801)
Cyclopentadiene	$1^1B_2(\pi \rightarrow \pi^*)$	5.26 (0.095)	5.31 (0.096)	5.34 (0.096)	5.32 (0.096)	5.27 (0.096)
	$2^1A_1(\pi \rightarrow \pi^*)$	7.10 (0.019)	7.39 (0.025)	7.70 (0.034)	8.12 (0.062)	8.27 (0.109)
	$3^1A_1(\pi \rightarrow \pi^*)$	8.29 (0.590)	8.34 (0.606)	8.38 (0.622)	8.41 (0.633)	8.41 (0.605)
Benzene	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.46 (0.000)	5.53 (0.000)	5.61 (0.000)	5.75 (0.000)	5.82
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.31 (0.000)	6.30 (0.000)	6.24 (0.000)	6.09 (0.000)	6.00
	$1^1E_{1u}(\pi \rightarrow \pi^*)$	7.19 (0.614)	7.27 (0.630)	7.35 (0.650)	7.47 (0.684)	7.52 (0.702)
	$2^1E_{2g}(\pi \rightarrow \pi^*)$	9.71	9.92	10.09	10.25	10.30
Pyrazine	$1^1B_{3u}(n \rightarrow \pi^*)$	4.18 (0.007)	4.32 (0.007)	4.48 (0.008)	4.72 (0.008)	4.84 (0.008)
	$1^1A_u(n \rightarrow \pi^*)$	4.94	5.23	5.60	6.25	6.61
	$1^1B_{2u}(n \rightarrow \pi^*)$	5.35 (0.098)	5.39 (0.107)	5.43 (0.118)	5.50 (0.138)	5.54 (0.148)
	$1^1B_{2g}(n \rightarrow \pi^*)$	5.84	5.97	6.10	6.30	6.39
	$1^1B_{1g}(n \rightarrow \pi^*)$	6.75	7.16	7.69	8.66	9.45
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.70 (0.079)	6.69 (0.075)	6.65 (0.066)	6.49 (0.048)	6.38 (0.040)
	$2^1B_{1u}(\pi \rightarrow \pi^*)$	7.88 (0.411)	7.95 (0.435)	8.02 (0.465)	8.10 (0.516)	8.12 (0.540)
	$2^1B_{2u}(\pi \rightarrow \pi^*)^a$	7.94 (0.364)	8.06 (0.376)	8.21 (0.387)	8.45 (0.403)	8.57 (0.412)
	$1^1B_{3g}(\pi \rightarrow \pi^*)^b$	9.92	10.34	10.76	10.95	11.02
	$2^1A_g(\pi \rightarrow \pi^*)$	8.64	9.03	9.49	10.18	10.41
Formaldehyde	$1^1A_2(n \rightarrow \pi^*)$	3.79	3.84	3.92	4.13	4.25
	$1^1B_1(\sigma \rightarrow \pi^*)$	8.40 (0.073)	8.74 (0.073)	9.16 (0.077)	9.82 (0.093)	10.12 (0.105)
	$2^1A_1(\pi \rightarrow \pi^*)^c$	9.51 (0.054)	9.56 (0.094)	9.57 (0.132)	9.50 (0.174)	9.41 (0.188)
Acetone	$1^1A_2(n \rightarrow \pi^*)$	4.32	4.38	4.48	4.71	4.86
	$1^1B_1(\sigma \rightarrow \pi^*)^d$	7.66 (0.028)	8.09 (0.029)	8.58 (0.031)	9.29 (0.033)	9.58 (0.036)
	$2^1A_1(\pi \rightarrow \pi^*)^e$	8.96 (0.162)	9.13 (0.211)	9.28 (0.248)	9.40 (0.281)	9.40 (0.288)
Acetamide	$1^1A''(n \rightarrow \pi^*)$	5.56 (0.001)	5.64 (0.001)	5.76 (0.001)	6.05 (0.001)	6.25 (0.001)
	$2^1A'(\pi \rightarrow \pi^*)$	7.58 (0.053)	7.85 (0.135)	8.09 (0.186)	8.47 (0.224)	8.65 (0.234)
	$3^1A'(\pi \rightarrow \pi^*)$	7.90 (0.181)	8.28 (0.121)	8.80 (0.090)	9.57 (0.077)	9.89 (0.077)

Table SI-4 (Continued.)

Molecule	State μ parameter	HF-srPBE(GWS)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
Cytosine	$2^1 A'(\pi \rightarrow \pi^*)$	5.02 (0.070)	5.16 (0.080)	5.32 (0.092)	5.58 (0.114)	5.71 (0.127)
	$1^1 A^\gamma(n \rightarrow \pi^*)$	5.24 (0.002)	5.45 (0.002)	5.71 (0.002)	6.17 (0.002)	6.44 (0.002)
	$2^1 A^\gamma(n \rightarrow \pi^*)$	5.86 (0.000)	6.00 (0.000)	6.17 (0.000)	6.55 (0.000)	6.80 (0.000)
	$3^1 A'(\pi \rightarrow \pi^*)$	6.01 (0.162)	6.24 (0.210)	6.49 (0.268)	6.87 (0.345)	7.06 (0.365)
	$4^1 A'(\pi \rightarrow \pi^*)$	6.78 (0.465)	6.91 (0.503)	7.08 (0.506)	7.40 (0.488)	7.58 (0.483)
	$5^1 A'(\pi \rightarrow \pi^*)$	7.11 (0.221)	7.40 (0.171)	7.78 (0.151)	8.38 (0.149)	8.68 (0.153)
Thymine	$6^1 A'(\pi \rightarrow \pi^*)$	7.95 (0.031)	8.44 (0.035)	9.00 (0.033)	9.63 (0.188)	9.83 (0.200)
	$1^1 A^\gamma(n \rightarrow \pi^*)$	5.05 (0.000)	5.19 (0.000)	5.35 (0.000)	5.67 (0.000)	5.88 (0.000)
	$2^1 A'(\pi \rightarrow \pi^*)$	5.29 (0.199)	5.43 (0.229)	5.59 (0.265)	5.83 (0.320)	5.92 (0.345)
	$3^1 A'(\pi \rightarrow \pi^*)$	6.75 (0.056)	6.98 (0.116)	7.24 (0.144)	7.65 (0.164)	7.85 (0.166)
	$2^1 A^\gamma(n \rightarrow \pi^*)$	6.36 (0.000)	6.48 (0.000)	6.65 (0.000)	7.01 (0.000)	7.25 (0.000)
	$4^1 A'(\pi \rightarrow \pi^*)$	6.80 (0.253)	7.11 (0.247)	7.47 (0.285)	8.00 (0.344)	8.25 (0.364)
	$3^1 A^\gamma(n \rightarrow \pi^*)$	7.04 (0.000)	7.28 (0.000)	7.54 (0.000)	7.85 (0.000)	7.91 (0.000)
	$4^1 A^\gamma(n \rightarrow \pi^*)$	7.35 (0.001)	7.88 (0.001)	8.39 (0.002)	8.86 (0.002)	8.92 (0.002)
	$5^1 A^\gamma(n \rightarrow \pi^*)$	7.53 (0.000)	8.00 (0.000)	8.54 (0.001)	9.04 (0.003)	9.19 (0.000)
Uracil	$5^1 A'(\pi \rightarrow \pi^*)$	7.81 (0.366)	8.04 (0.327)	8.34 (0.271)	8.89 (0.188)	9.18 (0.154)
	$1^1 A^\gamma(n \rightarrow \pi^*)$	5.02 (0.000)	5.16 (0.000)	5.33 (0.000)	5.66 (0.000)	5.87 (0.000)
	$2^1 A'(\pi \rightarrow \pi^*)$	5.47 (0.194)	5.61 (0.225)	5.76 (0.263)	6.00 (0.321)	6.10 (0.349)
	$3^1 A'(\pi \rightarrow \pi^*)$	6.70 (0.057)	7.02 (0.068)	7.33 (0.092)	7.77 (0.120)	7.98 (0.125)
	$2^1 A^\gamma(n \rightarrow \pi^*)$	6.28 (0.000)	6.42 (0.000)	6.59 (0.000)	6.95 (0.000)	7.19 (0.000)
	$3^1 A^\gamma(n \rightarrow \pi^*)$	7.24 (0.000)	7.49 (0.000)	7.75 (0.001)	8.07 (0.001)	8.12 (0.001)
	$4^1 A'(\pi \rightarrow \pi^*)$	6.98 (0.182)	7.23 (0.218)	7.56 (0.262)	8.10 (0.334)	8.36 (0.360)
	$4^1 A^\gamma(n \rightarrow \pi^*)$	7.34 (0.001)	7.82 (0.001)	8.34 (0.002)	9.06 (0.004)	9.24 (0.000)
	$5^1 A^\gamma(n \rightarrow \pi^*)$	7.42 (0.000)	7.93 (0.000)	8.55 (0.000)	9.19 (0.000)	9.38 (0.004)
Adenine	$5^1 A'(\pi \rightarrow \pi^*)$	7.74 (0.415)	7.95 (0.389)	8.23 (0.337)	8.78 (0.245)	9.07 (0.208)
	$2^1 A'(\pi \rightarrow \pi^*)$	5.43 (0.290)	5.55 (0.248)	5.67 (0.257)	5.84 (0.320)	5.90 (0.338)
	$3^1 A'(\pi \rightarrow \pi^*)$	5.47 (0.024)	5.59 (0.083)	5.73 (0.086)	5.94 (0.037)	6.04 (0.026)
	$1^1 A^\gamma(n \rightarrow \pi^*)$	5.31 (0.000)	5.56 (0.000)	5.86 (0.001)	6.38 (0.000)	6.66 (0.000)
	$2^1 A^\gamma(n \rightarrow \pi^*)$	5.95 (0.001)	6.18 (0.002)	6.45 (0.002)	6.89 (0.002)	7.11 (0.001)
	$4^1 A'(\pi \rightarrow \pi^*)$	6.70 (0.485)	6.85 (0.499)	7.01 (0.483)	7.25 (0.379)	7.34 (0.279)
	$5^1 A'(\pi \rightarrow \pi^*)$	7.06 (0.010)	7.26 (0.027)	7.43 (0.069)	7.65 (0.197)	7.74 (0.307)
	$6^1 A'(\pi \rightarrow \pi^*)$	7.13 (0.128)	7.31 (0.184)	7.51 (0.254)	7.79 (0.360)	7.92 (0.398)
$7^1 A'(\pi \rightarrow \pi^*)$	7.61 (0.160)	7.81 (0.146)	8.04 (0.127)	8.41 (0.102)	8.58 (0.094)	

Table SI-5: Ahlrichs TZVP, Dunning cc-pVTZ and aug-cc-pVTZ basis comparison with CAS-srPBE(HSE;RI). Linear response excitation energies for the various molecule in eV and oscillator strengths for allowed transitions in parenthesis. For CAS-srPBE(HSE;RI) the range separation parameter is taken to $\mu = 0.4$. Δ_{TZ} and Δ_{aTZ} are respectively the contribution of cc-pVTZ and aug-cc-pVTZ to TZVP, in bold face significant basis effects (> 0.4 eV). The complete active spaces (CAS) are specified for CAS-srPBE(HSE;RI).

Molecule	State	CAS-srPBE(HSE;RI) $\mu = 0.4$			Basis effects		CASPT2 ^a	
		TZVP	cc-pVTZ	aug-cc-pVTZ	Δ_{TZ}	Δ_{aTZ}	TZVP	aug-cc-pVTZ
<i>E</i> -Butadiene CAS(2 <i>a_u</i> , 2 <i>b_g</i>) ⁴	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	6.10 (0.731)	6.10 (0.715)	5.93 (0.694)	0.00	-0.17	6.47 (0.783)	6.38 (0.635)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	6.96	7.00	6.82	0.04	-0.14	6.62	6.43
all- <i>E</i> -Hexatriene CAS(1 <i>a_g</i> , 1 <i>b_u</i> , 3 <i>a_u</i> , 3 <i>b_g</i>) ⁸	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	5.10 (1.129)	5.07 (1.112)	4.98 (1.115)	-0.03	-0.12	5.31 (1.045)	5.18 (0.981)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	5.77	5.77	5.73	0.00	-0.04	5.42	5.33
all- <i>E</i> -Octatetraene CAS(4 <i>a_u</i> , 4 <i>b_g</i>) ⁸	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	4.88	4.89	4.88	0.01	0.00	4.64	4.52
	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	4.43 (1.504)	4.41 (1.532)	4.35 (1.543)	-0.03	-0.10	4.70 (1.299)	4.35 (1.307)
Cyclopentadiene CAS(2 <i>b₁</i> , 2 <i>a₂</i>) ⁴	1 ¹ <i>B₂</i> ($\pi \rightarrow \pi^*$)	5.39 (0.096)	5.36 (0.087)	5.29 (0.088)	-0.02	-0.10	5.51 (0.144)	5.43 (0.117)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	6.76 (0.009)	6.74 (0.009)	6.66 (0.003)	0.00	-0.39	6.31 (0.001)	6.28 (0.000)
	3 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^b	8.35 (0.580)	8.35 (0.536)	8.09 (0.396)	0.00	-0.26	8.52 (0.965)	8.15 (0.642)
Benzene CAS(1 <i>b_{1u}</i> , 1 <i>b_{2g}</i> , 1 <i>b_{3g}</i> , 1 <i>a_u</i>) ⁴	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.87	5.87	5.81	-0.01	-0.09	5.04	4.96
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.55	6.54	6.46	0.00	-0.15	6.42	6.57
	1 ¹ <i>E_{1u}</i> ($\pi \rightarrow \pi^*$)	7.28 (0.626)	7.28 (0.605)	7.13 (0.625)	-0.07	-0.34	7.13 (0.847)	7.36 (0.787)
	2 ¹ <i>E_{2g}</i> ($\pi \rightarrow \pi^*$)	9.21	9.14	8.87	-0.03	-0.05	8.18	8.15
Pyrazine CAS ^c	1 ¹ <i>B_{3u}</i> ($n \rightarrow \pi^*$)	4.21 (0.007)	4.18 (0.005)	4.16 (0.006)	-0.03	-0.02	4.12 (0.012)	4.02 (0.009)
	1 ¹ <i>A_u</i> ($n \rightarrow \pi^*$)	5.10	5.07	5.08	-0.02	-0.08	4.70	4.75
	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.68 (0.127)	5.66 (0.127)	5.60 (0.138)	0.00	-0.02	4.85 (0.123)	4.80 (0.127)
	1 ¹ <i>B_{2g}</i> ($n \rightarrow \pi^*$)	5.83	5.83	5.81	0.00	0.00	5.68	5.56
	1 ¹ <i>B_{1g}</i> ($n \rightarrow \pi^*$)	6.96	6.96	6.96	-0.04	-0.10	6.41	6.47
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.94 (0.094)	6.90 (0.096)	6.84 (0.080)	-0.03	-0.28	6.89 (0.107)	6.61 (0.176)
	2 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	7.94 (0.388)	7.91 (0.351)	7.66 (0.368)	-0.10	-0.19	7.79 (0.774)	7.71 (0.620)
	2 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$) ^d	8.17 (0.323)	8.07 (0.297)	7.98 (0.284)	-0.06	-0.32	7.66 (0.622)	7.73 (0.598)
	1 ¹ <i>B_{3g}</i> ($\pi \rightarrow \pi^*$) ^e	9.73	9.67	9.41	-0.17	-1.77	8.47	8.33
2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	8.96	8.79	8.53	0.02	-0.43	8.61	8.30	
Formaldehyde CAS(2 <i>a₁</i> , 2 <i>b₁</i> , 2 <i>b₂</i>) ⁶	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	3.84	3.86	3.82	-0.25	-1.46	3.99	4.01
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.57 (0.083)	8.32 (0.090)	7.11 (0.014)	-0.17	-1.26	9.14 (0.013)	9.12 (0.012)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^f	10.57 (0.319)	10.40 (0.343)	9.31 (0.133)	0.01	0.00	9.32 (0.451)	9.47 (0.242)
Acetone CAS(1 <i>a₁</i> , 1 <i>b₁</i> , 2 <i>b₂</i>) ²	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	4.32	4.33	4.32	0.04	-1.22	4.44	4.49
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.11 (0.030)	8.15(0.032)	6.89 (0.030)	-0.03	-0.14	9.27 (0.011)	9.25 (0.009)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^g	9.11 (0.212)	9.08 (0.183)	8.97 (0.256)	0.03	-0.05	9.31 (0.358)	9.19 (0.357)
Acetamide CAS(3 <i>a'</i> , 2 <i>a''</i>) ⁴	1 ¹ <i>A''</i> ($n \rightarrow \pi^*$)	5.59 (0.001)	5.62 (0.001)	5.54 (0.000)	0.05	-0.78	5.69 (0.001)	5.69 (0.002)
	2 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.65 (0.107)	7.70 (0.092)	6.87 (0.024)	0.00	0.00	7.27 (0.424)	7.12 (0.299)
	3 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	8.12 (0.145)	8.15 (0.138)	7.35 (0.171)	-0.03	0.77	10.09 (0.263)	10.03(0.164)

^a See Ref. 1

^b This cyclopentadiene state corresponds to 4¹*A₁*($\pi \rightarrow \pi^*$) for CAS-srPBE(HSE;RI) in aug-cc-pVTZ. ^c CAS(2*a_g*, 1*b_{3u}*, 1*b_{2u}*, 1*b_{1g}*, 1*b_{1u}*, 1*b_{2g}*, 1*b_{3g}*, 1*a_u*)⁶ for CAS-srPBE(HSE;RI).

^d This pyrazine state corresponds to 3¹*B_{2u}* for CAS-srPBE(HSE;RI) in aug-cc-pVTZ.

^e This pyrazine state corresponds to 2¹*B_{3g}* for CAS-srPBE(HSE;RI) in aug-cc-pVTZ.

^f This formaldehyde state corresponds to 4¹*A₁* CAS-srPBE(HSE;RI) in the three basis sets.

^g This acetone state corresponds to 4¹*A₁* for CAS-srPBE(HSE;RI) in aug-cc-pVTZ.

Table SI-5 (Continued.)

Molecule	State	CAS-srPBE(HSE;RI) $\mu = 0.4$			Basis effects		CASPT2 ^a	
		TZVP	cc-pVTZ	aug-cc-pVTZ	Δ_{TZ}	Δ_{aTZ}	TZVP	aug-cc-pVTZ
Cytosine CAS(4a', 6a'') ¹⁰	2 ¹ A'($\pi \rightarrow \pi^*$)	4.95 (0.061)	4.94 (0.058)	4.88 (0.060)	-0.01	-0.07	4.67 (0.093)	4.52 (0.053)
	1 ¹ A''($n \rightarrow \pi^*$)	5.24 (0.002)	5.08 (0.001)	5.05 (0.002)	-0.16	-0.19	5.12 (0.003)	5.03 (0.003)
	2 ¹ A''($n \rightarrow \pi^*$)	5.89 (0.000)	5.90 (0.000)	5.85 (0.000)	0.01	-0.04	5.53 (0.002)	5.44 (0.001)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.91 (0.127)	5.97 (0.129)	5.85 (0.139)	0.06	-0.06	5.53 (0.352)	5.43 (0.238)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.69 (0.489)	6.48 (0.331)	6.17 (0.300)	-0.21	-0.52	6.40 (0.623)	6.09 (0.546)
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.11 (0.222)	7.17 (0.212)	6.87 (0.094)	0.06	-0.24	6.97 (0.366)	6.68 (0.406)
Thymine CAS(6a', 6a'') ¹²	6 ¹ A'($\pi \rightarrow \pi^*$)	8.10 (0.023)	7.58 (0.143)	7.15 (0.254)	-0.52	-0.95	8.23 (0.132)	-
	1 ¹ A''($n \rightarrow \pi^*$)	4.97 (0.000)	5.11 (0.000)	4.98 (0.000)	0.14	0.01	4.95 (0.000)	4.86 (-)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.37 (0.195)	5.24 (0.165)	5.20 (0.107)	-0.13	-0.17	5.06 (0.334)	4.91 (0.278)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.65 (0.084)	6.64 (0.061)	5.70 (0.197)	-0.01	-0.95	6.15 (0.067)	6.01 (0.067)
	2 ¹ A''($n \rightarrow \pi^*$)	6.45 (0.000)	6.40 (0.000)	6.31 (0.001)	-0.05	-0.14	6.38 (0.000)	6.22 (-)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.69 (0.184)	6.76 (0.217)	6.56 (0.209)	0.07	-0.13	6.53 (0.356)	6.32 (0.283)
	3 ¹ A''($n \rightarrow \pi^*$)	7.28 (0.000)	7.23 (0.000)	6.39 (0.000)	-0.05	-0.89	6.85 (0.000)	6.59 (-)
	4 ¹ A''($n \rightarrow \pi^*$)	7.30 (0.000)	7.28 (0.000)	7.05 (0.001)	-0.02	-0.25	7.43 (0.000)	7.05 (-)
5 ¹ A''($n \rightarrow \pi^*$)	7.47 (0.000)	7.47 (0.000)	7.25 (0.000)	0.00	-0.22	-	-	
Uracil CAS(6a', 6a'') ¹²	5 ¹ A'($\pi \rightarrow \pi^*$)	7.63 (0.441)	7.83 (0.401)	6.72 (0.007)	0.20	-0.91	7.43 (0.672)	7.33 (0.680)
	1 ¹ A''($n \rightarrow \pi^*$)	4.93 (0.000)	4.95 (0.000)	4.94 (0.000)	0.02	0.01	4.91 (0.000)	4.80
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.53 (0.200)	5.48 (0.168)	5.39 (0.159)	-0.05	-0.14	5.23 (0.320)	5.06 (0.276)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.61 (0.055)	6.57 (0.077)	6.38 (0.171)	-0.04	-0.23	6.15 (0.047)	6.00 (0.045)
	2 ¹ A''($n \rightarrow \pi^*$)	6.38 (0.000)	6.40 (0.000)	6.33 (0.000)	0.02	-0.05	6.28 (0.000)	6.15
	3 ¹ A''($n \rightarrow \pi^*$)	7.21 (0.000)	7.24 (0.000)	6.55 (0.004)	0.03	-0.66	6.98 (0.000)	6.73
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.85 (0.146)	6.81 (0.142)	6.60 (0.102)	-0.04	-0.25	6.74 (0.249)	6.47 (0.259)
	4 ¹ A''($n \rightarrow \pi^*$)	7.46 (0.001)	7.41 (0.001)	7.18 (0.001)	-0.05	-0.28	7.28 (0.000)	6.93
5 ¹ A''($n \rightarrow \pi^*$)	7.50 (0.000)	7.48 (0.000)	7.41 (0.002)	-0.02	-0.09	-	-	
Adenine CAS(4a', 8a'') ¹²	5 ¹ A'($\pi \rightarrow \pi^*$)	7.64 (0.465)	7.30 (0.293)	6.93 (0.197)	-0.34	-0.71	7.43 (0.804)	7.37 (0.212)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.48 (0.271)	5.40 (0.186)	5.30 (0.210)	-0.08	-0.18	5.20 (0.146)	5.11 (0.398)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.54 (0.024)	5.52 (0.076)	5.48 (0.059)	-0.02	-0.06	5.29 (0.201)	5.02 (0.015)
	1 ¹ A''($n \rightarrow \pi^*$)	5.48 (0.001)	5.47 (0.000)	5.45 (0.001)	-0.01	-0.03	5.19 (0.001)	5.04 (0.002)
	2 ¹ A''($n \rightarrow \pi^*$)	6.03 (0.002)	6.03 (0.002)	5.99 (0.002)	0.00	-0.04	5.96 (0.002)	5.75 (0.007)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.49 (0.049)	6.04 (0.038)	5.93 (0.044)	-0.45	-0.56	6.34 (0.538)	6.25 (0.510)
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.76 (0.462)	6.73 (0.458)	6.59 (0.486)	-0.03	-0.17	6.64 (0.001)	6.65 (0.069)
	6 ¹ A'($\pi \rightarrow \pi^*$)	7.15 (0.081)	7.11 (0.047)	6.92 (0.011)	-0.04	-0.23	6.87 (0.010)	6.96 (0.344)
7 ¹ A'($\pi \rightarrow \pi^*$)	7.44 (0.232)	7.29 (0.074)	7.12 (0.172)	-0.15	-0.32	7.56 (0.037)	7.55 (0.036)	

^aData from publications by the Roos group in the 1990's found in 2.

Table SI-6: CAS-srPBE(HSE;RI): μ dependency and oscillator strengths for allowed transitions in parenthesis. The complete active spaces (CAS) are specified for CAS-srPBE(HSE;RI).

Molecule	State μ parameter	CAS-srPBE(HSE;RI)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
<i>E</i> -Butadiene CAS(2 <i>a_u</i> , 2 <i>b_g</i>) ⁴	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$) ^a	5.99 (0.705)	6.10 (0.731)	6.25 (0.760)	6.58 (0.800)	5.96 (0.614)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	6.91	6.96	7.01	7.06	6.59
all- <i>E</i> -Hexatriene CAS(1 <i>a_g</i> , 1 <i>b_u</i> , 3 <i>a_u</i> , 3 <i>b_g</i>) ⁸	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$) ^b	4.96 (1.094)	5.09 (1.129)	5.28 (1.169)	5.67 (1.227)	5.93 (1.250)
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	5.69	5.75	5.84	5.99	6.08
all- <i>E</i> -Octatetraene CAS(4 <i>a_u</i> , 4 <i>b_g</i>) ⁸	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	4.85	4.89	4.94	5.03	5.07
	1 ¹ <i>B_u</i> ($\pi \rightarrow \pi^*$)	4.32 (1.508)	4.44 (1.547)	4.63 (1.593)	3.18 (1.675)	5.34 (1.686)
Cyclopentadiene CAS(2 <i>b₁</i> , 2 <i>a₂</i>) ⁴	1 ¹ <i>B₂</i> ($\pi \rightarrow \pi^*$)	5.29 (0.095)	5.39 (0.096)	5.52 (0.096)	5.80 (0.093)	-
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	6.67 (0.010)	6.76 (0.009)	6.85 (0.007)	6.94 (0.003)	-
	3 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	8.24 (0.470)	8.35 (0.580)	8.48 (0.632)	8.71 (0.667)	-
Benzene CAS(1 <i>b_{1u}</i> , 1 <i>b_{2g}</i> , 1 <i>b_{3g}</i> , 1 <i>a_u</i>) ⁴	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.69	5.87	6.09	6.45	6.63
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.48	6.55	6.62	6.69	6.77
	1 ¹ <i>E_{1u}</i> ($\pi \rightarrow \pi^*$)	7.20 (0.610)	7.28 (0.626)	7.39 (0.646)	7.57 (0.679)	7.68 (0.689)
	2 ¹ <i>E_{2g}</i> ($\pi \rightarrow \pi^*$)	9.11	9.21	9.28	9.27	9.21
Pyrazine CAS ^c	1 ¹ <i>B_{3u}</i> ($n \rightarrow \pi^*$)	4.14 (0.007)	4.21 (0.007)	4.40 (0.007)	4.60 (0.008)	4.72 (0.022)
	1 ¹ <i>A_u</i> ($n \rightarrow \pi^*$)	4.91	5.10	5.56	6.32	6.80
	1 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	5.36 (0.093)	5.68 (0.127)	5.33 (0.097)	5.15 (0.087)	4.99 (0.074)
	1 ¹ <i>B_{2g}</i> ($n \rightarrow \pi^*$)	5.69	5.83	5.87	5.94	5.94
	1 ¹ <i>B_{1g}</i> ($n \rightarrow \pi^*$)	6.62	6.96	7.50	8.56	9.24
	1 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	6.73 (0.075)	6.94 (0.094)	6.84 (0.070)	6.93 (0.059)	7.03 (0.054)
	2 ¹ <i>B_{1u}</i> ($\pi \rightarrow \pi^*$)	7.86 (0.410)	7.94 (0.388)	8.01 (0.455)	8.17 (0.492)	8.31 (0.504)
	2 ¹ <i>B_{2u}</i> ($\pi \rightarrow \pi^*$)	7.90 (0.365)	8.17 (0.323)	8.09 (0.400)	8.25 (0.438)	8.37 (0.455)
	1 ¹ <i>B_{3g}</i> ($\pi \rightarrow \pi^*$)	9.31	9.73	9.28	9.06	8.87
	2 ¹ <i>A_g</i> ($\pi \rightarrow \pi^*$)	8.69	8.96	8.96	8.78	8.66
Formaldehyde CAS(2 <i>a₁</i> , 2 <i>b₁</i> , 2 <i>b₂</i>) ⁶	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	3.80	3.84	3.90	4.03	4.14
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	8.31 (0.081)	8.57 (0.083)	8.83 (0.086)	9.06 (0.086)	9.10 (0.086)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$) ^d	10.38 (0.335)	10.57 (0.319)	10.80 (0.319)	11.02 (0.300)	11.06 (0.310)
Acetone CAS(1 <i>a₁</i> , 1 <i>b₁</i> , 2 <i>b₂</i>) ²	1 ¹ <i>A₂</i> ($n \rightarrow \pi^*$)	4.28	4.32	4.35	4.40	4.41
	1 ¹ <i>B₁</i> ($\sigma \rightarrow \pi^*$)	7.69 (0.028)	8.11 (0.030)	8.59 (0.031)	9.31 (0.035)	9.63 (0.039)
	2 ¹ <i>A₁</i> ($\pi \rightarrow \pi^*$)	8.95 (0.162)	9.11 (0.212)	9.22 (0.249)	9.23 (0.282)	9.17 (0.293)
Acetamide CAS(3 <i>a'</i> , 2 <i>a''</i>) ⁴	1 ¹ <i>A''</i> ($n \rightarrow \pi^*$)	5.53 (0.001)	5.59 (0.001)	5.66 (0.001)	5.84 (0.001)	5.97 (0.001)
	2 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.42 (0.035)	7.65 (0.107)	7.91 (0.143)	8.38 (0.179)	8.58 (0.183)
	3 ¹ <i>A'</i> ($\pi \rightarrow \pi^*$)	7.81 (0.190)	8.12 (0.145)	8.50 (0.118)	8.96 (0.100)	9.04 (0.109)

^a For butadiene CAS-srPBE(HSE;RI) with $\mu \in \{0.33, 0.5, 1\}$, a triplet 1³*B_u* comes before the 1¹*B_u* state in the response function.

^b For hexatriene CAS-srPBE(HSE;RI) with $\mu = 0.75$, a triplet 1³*B_u* comes before the 1¹*B_u* state in the response function.

^c CAS(2*a_g*, 1*b_{3u}*, 1*b_{2u}*, 1*b_{1g}*, 1*b_{1u}*, 1*b_{2g}*, 1*b_{3g}*, 1*a_u*)⁶ for CAS-srPBE(HSE;RI).

^d This formaldehyde state corresponds to 4¹*A₁* for CAS-srPBE(HSE;RI).

Table SI-6 (Continued.)

Molecule	State μ parameter	CAS-srPBE(HSE;RI)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
Cytosine CAS(8a', 6a'') ¹²	2 ¹ A'($\pi \rightarrow \pi^*$)	4.84 (0.053)	4.95 (0.062)	5.11 (0.079)	5.25 (0.105)	5.27 (0.116)
	1 ¹ A''($n \rightarrow \pi^*$)	5.07 (0.002)	5.23 (0.002)	5.40 (0.002)	5.64 (0.002)	5.77 (0.002)
	2 ¹ A''($n \rightarrow \pi^*$)	5.64 (0.000)	5.88 (0.000)	6.13 (0.000)	6.58 (0.000)	6.85 (0.000)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.74 (0.120)	5.90 (0.127)	6.12 (0.112)	6.43 (0.089)	6.54 (0.068)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.64 (0.381)	6.67 (0.484)	6.88 (0.562)	7.13 (0.638)	7.25 (0.678)
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.89 (0.325)	7.09 (0.228)	7.40 (0.217)	7.93 (0.191)	8.21 (0.179)
Thymine CAS(6a', 6a'') ¹²	6 ¹ A'($\pi \rightarrow \pi^*$)	7.41 (0.025)	8.08 (0.021)	8.68 (0.153)	9.09 (0.184)	9.26 (0.188)
	1 ¹ A''($n \rightarrow \pi^*$)	4.87 (0.000)	4.97 (0.000)	5.30 (0.000)	5.70 (0.000)	5.16 (0.000)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.20 (0.172)	5.37 (0.195)	5.42 (0.183)	5.82 (0.283)	6.00 (0.332)
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.42 (0.096)	6.65 (0.084)	6.86 (0.134)	7.36 (0.087)	7.60 (0.086)
	2 ¹ A''($n \rightarrow \pi^*$)	6.27 (0.000)	6.45 (0.000)	6.49 (0.000)	6.42 (0.000)	6.44 (0.000)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.54 (0.140)	6.69 (0.184)	7.02 (0.279)	7.63 (0.331)	7.92 (0.356)
	3 ¹ A''($n \rightarrow \pi^*$)	6.93 (0.000)	7.28 (0.000)	7.58 (0.000)	7.87 (0.000)	7.88 (0.000)
	4 ¹ A''($n \rightarrow \pi^*$)	7.04 (0.000)	7.30 (0.000)	7.80 (0.000)	8.85 (0.001)	9.03 (0.000)
Uracil CAS(6a', 6a'') ¹²	5 ¹ A''($n \rightarrow \pi^*$)	7.07 (0.000)	7.47 (0.000)	7.99 (0.000)	8.89 (0.003)	9.11 (0.010)
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.24 (0.264)	7.63 (0.441)	7.87 (0.356)	8.64 (0.268)	8.84 (0.234)
	1 ¹ A''($n \rightarrow \pi^*$)	4.80 (0.000)	4.93 (0.000)	5.27 (0.000)	5.68 (0.000)	5.19 (0.000)
	2 ¹ A'($\pi \rightarrow \pi^*$)	3.33 (0.018)	5.53 (0.200)	5.59 (0.188)	5.87 (0.206)	6.40 (0.346)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.34 (0.153)	6.61 (0.055)	6.92 (0.059)	6.86 (0.283)	7.95 (0.110)
	2 ¹ A''($n \rightarrow \pi^*$)	6.14 (0.000)	6.38 (0.000)	6.43 (0.000)	6.52 (0.000)	6.41 (0.000)
	3 ¹ A''($n \rightarrow \pi^*$)	6.62 (0.000)	7.21 (0.000)	7.77 (0.001)	8.10 (0.001)	8.01 (0.001)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.37 (0.048)	6.85 (0.146)	7.09 (0.249)	7.24 (0.198)	8.28 (0.320)
Adenine CAS(4a', 8a'') ¹²	4 ¹ A''($n \rightarrow \pi^*$)	6.89 (0.000)	7.46 (0.001)	7.83 (0.000)	8.82 (0.002)	9.18 (0.000)
	5 ¹ A''($n \rightarrow \pi^*$)	7.23 (0.000)	7.50 (0.000)	7.86 (0.001)	9.26 (0.000)	9.35 (0.007)
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.73 (0.143)	7.64 (0.465)	7.79 (0.429)	8.28 (0.238)	8.91 (0.248)
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.33 (0.275)	5.53 (0.007)	5.62 (0.109)	5.60 (0.018)	5.48 (0.015)
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.43 (0.013)	5.46 (0.293)	5.67 (0.202)	5.92 (0.281)	5.90 (0.291)
	1 ¹ A''($n \rightarrow \pi^*$)	5.24 (0.000)	5.47 (0.001)	5.75 (0.000)	6.15 (0.002)	6.28 (0.003)
	2 ¹ A''($n \rightarrow \pi^*$)	5.84 (0.002)	6.00 (0.002)	6.24 (0.003)	6.54 (0.004)	6.67 (0.003)
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.58 (0.437)	6.70 (0.483)	6.89 (0.508)	7.10 (0.460)	6.95 (0.166)
Adenine CAS(4a', 8a'') ¹²	5 ¹ A'($\pi \rightarrow \pi^*$)	6.70 (0.005)	6.88 (0.013)	7.08 (0.033)	7.28 (0.120)	7.23 (0.415)
	6 ¹ A'($\pi \rightarrow \pi^*$)	6.96 (0.094)	7.14 (0.105)	7.37 (0.115)	7.66 (0.154)	7.76 (0.096)
	7 ¹ A'($\pi \rightarrow \pi^*$)	7.40 (0.211)	7.52 (0.219)	7.67 (0.263)	7.91 (0.241)	7.97 (0.289)

Table SI-7: HF-srPBE(HSE;RI) μ dependency and oscillator strengths for allowed transitions in parenthesis

Molecule	State μ parameter	HF-srPBE(HSE;RI)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
<i>E</i> -Butadiene	$1^1B_u(\pi \rightarrow \pi^*)$	6.01 (0.720)	6.07 (0.750)	6.12 (0.786)	6.13 (0.841)	6.10 (0.868)
	$2^1A_g(\pi \rightarrow \pi^*)$	7.77	8.00	8.09	8.10	8.08
all- <i>E</i> -Hexatriene	$1^1B_u(\pi \rightarrow \pi^*)$	5.03 (1.122)	5.11 (1.162)	5.17 (1.212)	5.20 (1.292)	5.19 (1.330)
	$2^1A_g(\pi \rightarrow \pi^*)$	7.00	7.21	7.26	7.29	7.29
all- <i>E</i> -Octatetraene	$2^1A_g(\pi \rightarrow \pi^*)$	6.26	6.39	6.47	6.52	6.52
	$1^1B_u(\pi \rightarrow \pi^*)$	4.40 (1.544)	4.49 (1.593)	4.56 (1.654)	4.59 (1.757)	4.58 (1.808)
Cyclopentadiene	$1^1B_2(\pi \rightarrow \pi^*)$	5.25 (0.094)	5.30 (0.095)	5.33 (0.095)	5.30 (0.095)	5.25 (0.095)
	$2^1A_1(\pi \rightarrow \pi^*)$	7.11 (0.020)	7.40 (0.026)	7.71 (0.035)	8.13 (0.065)	8.28 (0.110)
	$3^1A_1(\pi \rightarrow \pi^*)$	8.29 (0.587)	8.34 (0.604)	8.37 (0.622)	8.40 (0.631)	8.40 (0.601)
Benzene	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.46	5.53	5.61	5.76	5.83
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.29	6.28	6.22	6.06	5.98
	$1^1E_{1u}(\pi \rightarrow \pi^*)$	7.20 (0.612)	7.27 (0.629)	7.35 (0.650)	7.47 (0.685)	7.52 (0.703)
	$2^1E_{2g}(\pi \rightarrow \pi^*)$	9.70	9.91	10.08	10.25	10.31
Pyrazine	$1^1B_{3u}(n \rightarrow \pi^*)$	4.19 (0.007)	4.33 (0.007)	4.49 (0.008)	4.73 (0.008)	4.85 (0.008)
	$1^1A_u(n \rightarrow \pi^*)$	4.96	5.25	5.62	6.27	6.63
	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.34 (0.098)	5.38 (0.106)	5.42 (0.118)	5.49 (0.139)	5.53 (0.149)
	$1^1B_{2g}(n \rightarrow \pi^*)$	5.84	5.98	6.12	6.32	6.42
	$1^1B_{1g}(n \rightarrow \pi^*)$	6.77	7.18	9.47	8.69	9.22
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.68 (0.076)	6.68 (0.072)	6.63 (0.064)	6.46 (0.047)	6.34 (0.039)
	$2^1B_{1u}(\pi \rightarrow \pi^*)$	7.88 (0.412)	7.95 (0.437)	8.02 (0.468)	8.10 (0.517)	8.11 (0.541)
	$2^1B_{2u}(\pi \rightarrow \pi^*)$	7.94 (0.362)	8.06 (0.375)	8.21 (0.385)	8.46 (0.403)	8.57 (0.410)
	$1^1B_{3g}(\pi \rightarrow \pi^*)$	9.91	10.66	10.74	10.94	11.00
	$2^1A_g(\pi \rightarrow \pi^*)$	8.70	9.07	9.50	10.14	10.38
Formaldehyde	$1^1A_2(n \rightarrow \pi^*)$	3.81	3.86	3.95	4.16	4.29
	$1^1B_1(\sigma \rightarrow \pi^*)$	8.42 (0.075)	8.75 (0.075)	9.14 (0.077)	9.77 (0.089)	10.11 (0.096)
	$2^1A_1(\pi \rightarrow \pi^*)^a$	9.49 (0.056)	9.94 (0.316)	9.54 (0.132)	9.47 (0.174)	9.47 (0.192)
Acetone	$1^1A_2(n \rightarrow \pi^*)$	4.32	4.39	4.49	4.73	4.88
	$1^1B_1(\sigma \rightarrow \pi^*)$	7.68 (0.028)	9.81 (0.026)	8.56 (0.031)	9.23 (0.034)	9.51 (0.038)
	$2^1A_1(\pi \rightarrow \pi^*)$	8.96 (0.159)	9.13 (0.209)	9.27 (0.245)	9.38 (0.278)	9.39 (0.285)
Acetamide	$1^1A''(n \rightarrow \pi^*)$	5.56 (0.001)	5.64 (0.001)	5.77 (0.001)	6.08 (0.001)	6.28 (0.001)
	$2^1A'(\pi \rightarrow \pi^*)$	7.59 (0.053)	7.85 (0.132)	8.10 (0.184)	8.48 (0.222)	8.66 (0.232)
	$3^1A'(\pi \rightarrow \pi^*)$	7.91 (0.180)	8.27 (0.123)	8.76 (0.092)	9.50 (0.080)	9.83 (0.078)

^a This formaldehyde state corresponds to 3^1A_1 for HF-srPBE(HSE;RI).

Table SI-7 (*Continued.*)

Molecule	State μ parameter	HF-srPBE(HSE;RI)				
		$\mu = 0.33$	$\mu = 0.4$	$\mu = 0.5$	$\mu = 0.75$	$\mu = 1.0$
Cytosine	$2^1A'(\pi \rightarrow \pi^*)$	5.03 (0.070)	5.17 (0.080)	5.33 (0.092)	5.59 (0.115)	5.72 (0.129)
	$1^1A''(n \rightarrow \pi^*)$	5.24 (0.002)	5.46 (0.004)	5.72 (0.002)	6.20 (0.002)	6.47 (0.002)
	$2^1A''(n \rightarrow \pi^*)$	5.86 (0.000)	6.00 (0.000)	6.18 (0.000)	6.58 (0.000)	6.84 (0.000)
	$3^1A'(\pi \rightarrow \pi^*)$	6.03 (0.163)	6.25 (0.212)	6.50 (0.271)	6.89 (0.345)	7.08 (0.363)
	$4^1A'(\pi \rightarrow \pi^*)$	6.79 (0.470)	6.93 (0.505)	7.10 (0.505)	7.42 (0.487)	7.60 (0.482)
	$5^1A'(\pi \rightarrow \pi^*)$	7.13 (0.213)	7.43 (0.168)	7.80 (0.150)	8.41 (0.149)	8.70 (0.154)
Thymine	$6^1A'(\pi \rightarrow \pi^*)^a$	7.93 (0.029)	8.90 (0.217)	8.96 (0.034)	9.63 (0.174)	9.83 (0.195)
	$1^1A''(n \rightarrow \pi^*)$	5.04 (0.000)	5.18 (0.000)	5.35 (0.000)	5.69 (0.000)	5.91 (0.000)
	$2^1A'(\pi \rightarrow \pi^*)$	5.30 (0.200)	5.45 (0.231)	5.60 (0.267)	5.83 (0.322)	5.93 (0.346)
	$3^1A'(\pi \rightarrow \pi^*)$	6.76 (0.057)	7.00 (0.105)	7.26 (0.134)	7.68 (0.157)	7.88 (0.161)
	$2^1A''(n \rightarrow \pi^*)$	6.35 (0.000)	6.49 (0.000)	6.66 (0.000)	7.04 (0.000)	7.29 (0.000)
	$4^1A'(\pi \rightarrow \pi^*)$	6.82 (0.251)	7.13 (0.258)	7.49 (0.293)	8.03 (0.349)	8.28 (0.367)
	$3^1A''(n \rightarrow \pi^*)$	7.04 (0.000)	7.28 (0.000)	7.53 (0.000)	7.81 (0.000)	7.87 (0.000)
	$4^1A''(n \rightarrow \pi^*)$	7.36 (0.000)	7.89 (0.001)	8.40 (0.002)	8.80 (0.002)	8.84 (0.002)
	$5^1A''(n \rightarrow \pi^*)$	7.53 (0.000)	8.30 (0.000)	8.53 (0.001)	9.05 (0.003)	9.14 (0.000)
Uracil	$5^1A'(\pi \rightarrow \pi^*)$	7.82 (0.367)	8.05 (0.327)	8.36 (0.271)	8.92 (0.189)	9.20 (0.154)
	$1^1A''(n \rightarrow \pi^*)$	5.01 (0.000)	5.16 (0.000)	5.33 (0.000)	5.68 (0.000)	5.90 (0.000)
	$2^1A'(\pi \rightarrow \pi^*)$	5.48 (0.195)	5.61 (0.227)	5.77 (0.264)	6.00 (0.323)	6.11 (0.350)
	$3^1A'(\pi \rightarrow \pi^*)$	6.71 (0.057)	7.03 (0.069)	7.35 (0.090)	7.80 (0.117)	8.00 (0.122)
	$2^1A''(n \rightarrow \pi^*)$	6.28 (0.000)	6.43 (0.000)	6.60 (0.000)	6.98 (0.000)	7.23 (0.000)
	$3^1A''(n \rightarrow \pi^*)$	7.24 (0.000)	7.49 (0.000)	7.74 (0.001)	8.02 (0.001)	8.08 (0.001)
	$4^1A'(\pi \rightarrow \pi^*)$	7.00 (0.181)	7.25 (0.217)	7.59 (0.264)	8.13 (0.335)	8.38 (0.360)
	$4^1A''(n \rightarrow \pi^*)$	7.34 (0.001)	7.83 (0.001)	8.35 (0.002)	9.07 (0.004)	9.19 (0.000)
	$5^1A''(n \rightarrow \pi^*)$	7.42 (0.000)	7.93 (0.000)	8.55 (0.000)	9.14 (0.000)	9.40 (0.004)
Adenine	$5^1A'(\pi \rightarrow \pi^*)$	7.75 (0.415)	7.96 (0.388)	8.25 (0.336)	8.80 (0.246)	9.09 (0.209)
	$2^1A'(\pi \rightarrow \pi^*)$	5.44 (0.275)	5.60 (0.092)	5.67 (0.256)	5.84 (0.323)	5.89 (0.341)
	$3^1A'(\pi \rightarrow \pi^*)$	5.47 (0.038)	5.55 (0.237)	5.74 (0.086)	5.94 (0.033)	6.05 (0.025)
	$1^1A''(n \rightarrow \pi^*)$	5.31 (0.000)	5.56 (0.000)	5.87 (0.000)	6.40 (0.000)	6.68 (0.000)
	$2^1A''(n \rightarrow \pi^*)$	5.95 (0.001)	6.18 (0.002)	6.46 (0.002)	6.91 (0.002)	7.14 (0.001)
	$4^1A'(\pi \rightarrow \pi^*)$	6.70 (0.484)	6.85 (0.496)	7.02 (0.478)	7.25 (0.365)	7.33 (0.257)
	$5^1A'(\pi \rightarrow \pi^*)$	7.07 (0.012)	7.26 (0.029)	7.44 (0.072)	7.64 (0.210)	7.74 (0.328)
	$6^1A'(\pi \rightarrow \pi^*)$	7.14 (0.130)	7.32 (0.189)	7.51 (0.261)	7.80 (0.363)	7.93 (0.399)
	$7^1A'(\pi \rightarrow \pi^*)$	7.62 (0.159)	7.82 (0.145)	8.05 (0.126)	8.42 (0.100)	8.59 (0.093)

^a This cytosine state corresponds to $7^1A'$ for HF-srPBE(HSE;RI) with $\mu = 0.4$.

Table SI-8: Comparison of the different exchange correlation functionals GWS and HSE;RI with CAS-srPBE ($\mu = 0.4$) in Ahlrichs TZVP, Dunning cc-pVTZ and aug-cc-pVTZ basis. Linear response excitation energies for the various molecule in eV and oscillator strengths for allowed transitions in parenthesis.

Molecule	State	CAS-srPBE $\mu = 0.4$					
		TZVP		cc-pVTZ		aug-cc-pVTZ	
Functional		GWS	HSE;RI	GWS	HSE;RI	GWS	HSE;RI
<i>E</i> -Butadiene	$1^1B_u(\pi \rightarrow \pi^*)$	6.10 (0.731)	6.10 (0.731)	6.10 (0.714)	6.10 (0.715)	5.93 (0.695)	5.93 (0.694)
CAS($2a_u, 2b_g$) ⁴	$2^1A_g(\pi \rightarrow \pi^*)$	6.94	6.96	6.98	7.00	6.81	6.82
all- <i>E</i> -Hexatriene	$1^1B_u(\pi \rightarrow \pi^*)$	5.09 (1.128)	5.10 (1.129)	5.07 (1.111)	5.07 (1.112)	4.98 (1.114)	4.98 (1.115)
CAS($1a_g, 1b_u, 3a_u, 3b_g$) ⁸	$2^1A_g(\pi \rightarrow \pi^*)$	5.73	5.77	5.75	5.77	5.71	5.73
all- <i>E</i> -Octatetraene	$2^1A_g(\pi \rightarrow \pi^*)$	4.87	4.88	4.88	4.89	4.86	4.88
CAS($4a_u, 4b_g$) ⁸	$1^1B_u(\pi \rightarrow \pi^*)$	4.43 (1.489)	4.43 (1.504)	4.41 (1.530)	4.41 (1.532)	4.35 (1.541)	4.35 (1.543)
Cyclopentadiene	$1^1B_2(\pi \rightarrow \pi^*)$	5.40 (0.096)	5.39 (0.096)	5.36 (0.088)	5.36 (0.087)	5.30 (0.089)	5.29 (0.088)
CAS($2b_1, 2a_2$) ⁴	$2^1A_1(\pi \rightarrow \pi^*)$	6.75 (0.009)	6.76 (0.009)	6.73 (0.009)	6.74 (0.009)	6.65 (0.003)	6.66 (0.003)
	$3^1A_1(\pi \rightarrow \pi^*)$	8.35 (0.576)	8.35 (0.580)	8.34 (0.527)	8.35 (0.536)	8.03 (0.407)	8.09 (0.396)
Benzene	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.87	5.87	5.87	5.87	5.82	5.81
CAS($1b_{1u}, 1b_{2g}, 1b_{3g}, 1a_u$) ⁴	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.57	6.55	6.55	6.54	6.48	6.46
	$1^1E_{1u}(\pi \rightarrow \pi^*)$	7.28 (0.627)	7.28 (0.626)	7.27 (0.605)	7.28 (0.605)	7.13 (0.624)	7.13 (0.625)
	$2^1E_{2g}(\pi \rightarrow \pi^*)$	9.20	9.21	9.13	9.14	8.98	8.87
Pyrazine	$1^1B_{3u}(n \rightarrow \pi^*)$	4.18 (0.007)	4.21 (0.007)	4.17 (0.005)	4.18 (0.005)	4.15 (0.006)	4.16 (0.006)
CAS ^a	$1^1A_u(n \rightarrow \pi^*)$	5.07	5.10	5.05	5.07	5.06	5.08
	$1^1B_{2u}(\pi \rightarrow \pi^*)$	5.69 (0.127)	5.68 (0.127)	5.67 (0.127)	5.66 (0.127)	5.61 (0.137)	5.60 (0.138)
	$1^1B_{2g}(n \rightarrow \pi^*)$	5.83	5.83	5.82	5.83	5.80	5.81
	$1^1B_{1g}(n \rightarrow \pi^*)$	6.93	6.96	6.93	6.96	6.93	6.96
	$1^1B_{1u}(\pi \rightarrow \pi^*)$	6.96 (0.098)	6.94 (0.094)	6.91 (0.099)	6.90 (0.096)	6.86 (0.085)	6.84 (0.080)
	$2^1B_{1u}(\pi \rightarrow \pi^*)$	7.94 (0.391)	7.94 (0.388)	7.91 (0.348)	7.91 (0.351)	7.71 (0.418)	7.66 (0.368)
	$2^1B_{2u}(\pi \rightarrow \pi^*)$	8.07 (0.311)	8.17 (0.323)	8.07 (0.298)	8.07 (0.297)	7.99 (0.279)	7.98 (0.284)
	$1^1B_{3g}(\pi \rightarrow \pi^*)$	9.72	9.73	9.65	9.67	9.47	9.41
	$2^1A_g(\pi \rightarrow \pi^*)$	8.92	8.96	8.84	8.79	8.63	8.53
Formaldehyde	$1^1A_2(n \rightarrow \pi^*)$	3.81	3.84	3.83	3.86	3.80	3.82
CAS($2a_1, 2b_1, 2b_2$) ⁶	$1^1B_1(\sigma \rightarrow \pi^*)$	8.56 (0.082)	8.57 (0.083)	8.33 (0.090)	8.32 (0.090)	7.21 (0.017)	7.11 (0.014)
	$2^1A_1(\pi \rightarrow \pi^*)$	10.57 (0.320)	10.57 (0.319)	10.41 (0.344)	10.40 (0.343)	9.35 (0.137)	9.31 (0.133)
Acetone	$1^1A_2(n \rightarrow \pi^*)$	4.31	4.32	4.33	4.33	4.31	4.32
CAS($1a_1, 1b_1, 2b_2$) ²	$1^1B_1(\sigma \rightarrow \pi^*)$	8.11 (0.029)	8.11 (0.030)	8.16 (0.032)	8.15(0.032)	7.00 (0.030)	6.89 (0.030)
	$2^1A_1(\pi \rightarrow \pi^*)$	9.12 (0.214)	9.11 (0.212)	9.08 (0.186)	9.08 (0.183)	8.99 (0.264)	8.97 (0.256)
Acetamide	$1^1A''(n \rightarrow \pi^*)$	5.59 (0.001)	5.59 (0.001)	5.62 (0.001)	5.62 (0.001)	5.53 (0.000)	5.54 (0.000)
CAS($3a', 2a''$) ⁴	$2^1A'(\pi \rightarrow \pi^*)$	7.64 (0.109)	7.65 (0.107)	7.70 (0.095)	7.70 (0.092)	6.96 (0.024)	6.87 (0.024)
	$3^1A'(\pi \rightarrow \pi^*)$	8.12 (0.143)	8.12 (0.145)	8.16 (0.135)	8.15 (0.138)	7.39 (0.186)	7.35 (0.171)

^b CAS($2a_g, 1b_{3u}, 1b_{2u}, 1b_{1g}, 1b_{1u}, 1b_{2g}, 1b_{3g}, 1a_u$)⁶ for CAS-srPBE.

Table SI-8 (Continued.)

Molecule	State	CAS-srPBE $\mu = 0.4$							
		TZVP		cc-pVTZ		aug-cc-pVTZ			
Functional		GWS	HSE;RI	GWS	HSE;RI	GWS	HSE;RI	GWS	HSE;RI
Cytosine CAS(4a', 6a'') ¹⁰	2 ¹ A'($\pi \rightarrow \pi^*$)	4.93 (0.061)	4.95 (0.061)	4.93 (0.058)	4.94 (0.058)	4.88 (0.060)	4.87 (0.060)		
	1 ¹ A''($n \rightarrow \pi^*$)	5.06 (0.002)	5.24 (0.002)	5.08 (0.001)	5.08 (0.001)	5.05 (0.002)	5.05 (0.002)		
	2 ¹ A''($n \rightarrow \pi^*$)	5.83 (0.000)	5.89 (0.000)	5.90 (0.000)	5.90 (0.000)	5.85 (0.000)	5.85 (0.000)		
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.95 (0.128)	5.91 (0.127)	5.95 (0.126)	5.97 (0.129)	5.85 (0.139)	5.84 (0.136)		
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.62 (0.460)	6.69 (0.489)	6.49 (0.341)	6.48 (0.331)	6.17 (0.300)	6.18 (0.311)		
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.10 (0.273)	7.11 (0.222)	7.14 (0.221)	7.17 (0.212)	6.87 (0.094)	6.86 (0.108)		
	6 ¹ A'($\pi \rightarrow \pi^*$)	8.35 (0.067)	8.10 (0.023)	7.61 (0.126)	7.58 (0.143)	7.15 (0.254)	7.18 (0.271)		
Thymine CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.98 (0.000)	4.97 (0.000)	5.12 (0.000)	5.11 (0.000)	4.98 (0.000)	4.98 (0.000)		
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.36 (0.193)	5.37 (0.195)	5.23 (0.164)	5.24 (0.165)	5.20 (0.107)	5.18 (0.095)		
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.64 (0.079)	6.65 (0.084)	6.63 (0.060)	6.64 (0.061)	5.70 (0.197)	5.63 (0.201)		
	2 ¹ A''($n \rightarrow \pi^*$)	6.44 (0.000)	6.45 (0.000)	6.39 (0.000)	6.40 (0.000)	6.31 (0.001)	6.38 (0.000)		
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.66 (0.192)	6.69 (0.184)	6.73 (0.218)	6.76 (0.217)	6.56 (0.209)	6.54 (0.212)		
	3 ¹ A''($n \rightarrow \pi^*$)	7.28 (0.000)	7.28 (0.000)	7.22 (0.000)	7.23 (0.000)	6.39 (0.000)	6.40 (0.000)		
	4 ¹ A''($n \rightarrow \pi^*$)	7.30 (0.000)	7.30 (0.000)	7.29 (0.000)	7.28 (0.000)	7.05 (0.001)	7.13 (0.001)		
	5 ¹ A''($n \rightarrow \pi^*$)	7.47 (0.000)	7.47 (0.000)	7.46 (0.000)	7.47 (0.000)	7.25 (0.000)	7.31 (0.001)		
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.61 (0.439)	7.63 (0.441)	7.82 (0.401)	7.83 (0.401)	6.72 (0.007)	6.70 (0.006)		
Uracil CAS(6a', 6a'') ¹²	1 ¹ A''($n \rightarrow \pi^*$)	4.93 (0.000)	4.93 (0.000)	4.95 (0.000)	4.95 (0.000)	4.94 (0.000)	4.94 (0.000)		
	2 ¹ A'($\pi \rightarrow \pi^*$)	5.52 (0.199)	5.53 (0.200)	5.47 (0.166)	5.48 (0.168)	5.39 (0.159)	5.38 (0.157)		
	3 ¹ A'($\pi \rightarrow \pi^*$)	6.60 (0.056)	6.61 (0.055)	6.55 (0.078)	6.57 (0.077)	6.38 (0.171)	6.36 (0.175)		
	2 ¹ A''($n \rightarrow \pi^*$)	6.38 (0.000)	6.38 (0.000)	6.39 (0.000)	6.40 (0.000)	6.33 (0.000)	6.32 (0.000)		
	3 ¹ A''($n \rightarrow \pi^*$)	7.20 (0.000)	7.21 (0.000)	7.23 (0.000)	7.24 (0.000)	6.55 (0.004)	6.63 (0.004)		
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.83 (0.146)	6.85 (0.146)	6.78 (0.142)	6.81 (0.142)	6.60 (0.102)	6.58 (0.099)		
	4 ¹ A''($n \rightarrow \pi^*$)	7.46 (0.001)	7.46 (0.001)	7.42 (0.001)	7.41 (0.001)	7.18 (0.001)	7.17 (0.001)		
	5 ¹ A''($n \rightarrow \pi^*$)	7.50 (0.000)	7.50 (0.000)	7.47 (0.000)	7.48 (0.000)	7.41 (0.002)	7.41 (0.000)		
	5 ¹ A'($\pi \rightarrow \pi^*$)	7.63 (0.466)	7.64 (0.465)	7.27 (0.283)	7.30 (0.293)	6.93 (0.197)	6.90 (0.191)		
Adenine CAS(4a', 8a'') ¹²	2 ¹ A'($\pi \rightarrow \pi^*$)	5.47 (0.266)	5.48 (0.271)	5.42 (0.226)	5.40 (0.186)	5.30 (0.210)	5.31 (0.235)		
	3 ¹ A'($\pi \rightarrow \pi^*$)	5.54 (0.027)	5.54 (0.024)	5.52 (0.047)	5.52 (0.076)	5.48 (0.059)	5.48 (0.043)		
	1 ¹ A''($n \rightarrow \pi^*$)	5.48 (0.001)	5.48 (0.001)	5.46 (0.000)	5.47 (0.000)	5.45 (0.001)	5.44 (0.001)		
	2 ¹ A''($n \rightarrow \pi^*$)	6.03 (0.002)	6.03 (0.002)	6.03 (0.002)	6.03 (0.002)	5.99 (0.002)	5.98 (0.002)		
	4 ¹ A'($\pi \rightarrow \pi^*$)	6.36 (0.037)	6.49 (0.049)	6.21 (0.032)	6.04 (0.038)	5.93 (0.044)	6.10 (0.045)		
	5 ¹ A'($\pi \rightarrow \pi^*$)	6.74 (0.480)	6.76 (0.462)	6.72 (0.447)	6.73 (0.458)	6.59 (0.486)	6.59 (0.470)		
	6 ¹ A'($\pi \rightarrow \pi^*$)	7.14 (0.072)	7.15 (0.081)	7.12 (0.063)	7.11 (0.047)	6.92 (0.011)	6.96 (0.032)		
	7 ¹ A'($\pi \rightarrow \pi^*$)	7.37 (0.190)	7.44 (0.232)	7.33 (0.181)	7.29 (0.074)	7.12 (0.172)	7.18 (0.208)		

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