Table 8.1. Position (ΔE in μm^{-1}) and intensity (f) of calculated and experimental (in vapor phase) excited states of naphthalene.

ΔE (f)							
Calculated						Experimental	
CIS(FC) 6-31+G(d)	TD-HF 6-31+G(d)	TD-DFT B3LYP/6-31+G(d)	CNDO/S (48 conf.) [(a)]	CNDOL (48 conf.) [(a)]	ZINDO/S (63 conf.) [(a)]	Absorption (vapor) [(b)]	Neon matrix [(c)]
4.16(0.090)	3.91(0.015)	3.55(0.009)	3.54(0.006)	3.34	3.26(0.006)	3.20(0.002)	3.21(0.07)
4.29	4.12	3.63	3.91(0.101)	3.89	3.72(0.162)	3.75(0.102)	3.58(0.13)
5.00	4.99	4.41	4.36	3.90	4.46		
5.20	5.08	4.44	4.44	3.92(0.001)	4.60(1.956)	4.75(1.0)	4.73(1.72)
5.30	5.29	4.66	4.74	3.93(0.028)	4.62		
5.32	5.29(0.301)	4.73	4.76	3.96	4.91(0.676)	4.95(0.3)	4.91(0.60)
5.60(2.154)	5.31	4.96	4.78(0.902)	4.24(0.002)	5.05		
5.62(0.062)	5.50(0.094)	5.02(0.003)	4.86	4.46	5.22	5.26(0.1)	
			4.87	4.50			
			5.03	4.60			
			5.18(0.357)	4.63			
			5.25	4.81			
				4.91			
				4.93(0.018)			
				5.02			
				5.18			
				5.28			

[(a)] Number of configurations included in the CIS calculation; [(b)] Ref. 4c; [(c)] Ref. 4f

Table 8.2. ZINDO/S calculations on naphthalene.

This work (MEE = 13eV) (63 Conf.) [a]							Ref. 7b, c (50-70 Conf.) [a]		Ref. 7e (Full-CIS) (1153 Conf.) [a]		Experiment [d]	
State	Configurations	Conf.[b]	(c^2)	Type	λ (nm)	ΔE [c] (f)	State	ΔE [c] (f)	State	ΔE [c] (f)	State	ΔE [c] (f)
$^1B_{2u}$	$1a_u \rightarrow 2b_{2g}$ $2b_{3u} \rightarrow 2b_{1g}$	H-L1 H1-L	(0.55) (0.43)	$\pi\pi^*$	307.2	3.26(0.006)	$^1B_{2u}$	3.25(0.002)	$^1B_{3u}$	3.23(0.003)	$^1B_{2u}$	3.20(0.002)
$^1B_{1u}$	$1a_u \rightarrow 2b_{1g}$	H-L	(0.88)	$\pi\pi^*$	268.6	3.72(0.162)	$^1B_{1u}$	3.77(0.148)	$^1B_{2u}$	3.39(0.166)	$^1B_{1u}$	3.75(0.102)
^1A_g	$2b_{3u} \rightarrow 3b_{3u}$ $1b_{2g} \rightarrow 2b_{2g}$	H1-L2 H2-L1	(0.56) (0.28)	$\pi\pi^*$	224.1	4.46	^1A_g	4.48	$^1B_{3u}$	4.28(1.590)		
$^1B_{2u}$	$1a_u \rightarrow 2b_{2g}$ $2b_{3u} \rightarrow 2b_{1g}$	H-L1 H1-L	(0.42) (0.55)	$\pi\pi^*$	217.5	4.60(1.956)	$^1B_{2u}$	4.58(1.866)	$^1B_{1g}$	4.29	$^1B_{2u}$	4.75(1.0)
$^1B_{3g}$	$1a_u \rightarrow 3b_{3u}$	H-L2	(0.80)	$\pi\pi^*$	216.6	4.62	$^1B_{3g}$	4.67	^1A_g	4.45		
$^1B_{1u}$	$2b_{3u} \rightarrow 2b_{2g}$	H1-L1	(0.87)	$\pi\pi^*$	203.7	4.91(0.676)	$^1B_{1u}$	4.86(0.672)	$^1B_{2u}$	4.53(0.563)	$^1B_{1u}$	4.95(0.3)
$^1B_{1g}$	$1a_u \rightarrow 5b_{1u}$	H-L4	(0.95)	$\pi\sigma^*$	198.1	5.05	$^1B_{1g}$	5.27	$^1B_{3g}$	4.93		
$^1B_{3g}$	$1b_{2g} \rightarrow 2b_{1g}$	H2-L	(0.96)	$\pi\pi^*$	191.5	5.22	$^1B_{3g}$	5.27	$^1B_{1g}$	4.95	$^1B_{2u}$	5.26(0.1)

[a] Number of configurations included in the CIS calculation; [b] Dominant configurations of each CIS state; [c] Units are μm^{-1}; [d] Ref. 4c

Table 8.3. ZINDO/S excited states of naphthalene using various energy criteria for the selection of the singly excited configurations.

MEE [(a)] (eV)	9.0	9.5	10.0	10.5	11.0	11.5	12.0
# Conf. [(b)]	7	11	11	17	23	29	41
ΔE (f) (in μm^{-1})	3.31 (0.002)	3.31 (0.002)	3.31 (0.002)	3.31 (0.002)	3.31 (0.002)	3.30 (0.004)	3.30 (0.004)
	3.89 (0.501)	3.75 (0.185)	3.75 (0.185)	3.75 (0.185)	3.75 (0.185)	3.75 (0.185)	3.74 (0.163)
	4.64 (2.068)	4.64 (2.068)	4.64 (2.068)	4.62	4.53	4.53	4.46
		4.64	4.64	4.64 (2.068)	4.62	4.60 (1.968)	4.60 (1.968)
		4.95 (0.932)	4.95 (0.932)	4.89	4.64 (2.068)	4.62	4.62
				4.95 (0.932)	4.95 (0.932)	4.95 (0.932)	4.91 (0.676)
				5.23	5.09	5.09	5.05
					5.23	5.23	5.23

MEE [(a)] (eV)	13.0	14.0	15.0	16.0	15-15 [(c)]	20-20 [(c)]
# Conf. [(b)]	63	85	123	171	451	801
ΔE (f) (in μm^{-1})	3.26 (0.006)	3.22 (0.003)	3.21 (0.003)	3.21 (0.003)	3.21 (0.003)	3.21 (0.004)
	3.72 (0.162)	3.72 (0.161)	3.71 (0.163)	3.70 (0.164)	3.65 (0.183)	3.53 (0.176)
	4.46	4.46	4.46	4.46	4.41 (1.711)	4.33 (1.723)
	4.60 (1.956)	4.60 (1.966)	4.54 (1.837)	4.53 (1.833)	4.46	4.43
	4.62	4.62	4.62	4.61	4.53	4.45
	4.91 (0.676)	4.91 (0.677)	4.86 (0.646)	4.86 (0.643)	4.71 (0.623)	4.61 (0.630)
	5.05	4.98	4.98	4.94	4.92	4.91
	5.22	5.22	5.22	5.21	5.09	5.01

[(a)] Maximum excitation energy; [(b)] Number of configurations considered; [(c)] Occupied and unoccupied MOs included in the production of singly excited determinants