

Data from Tozer's Benchmark Set. Row 1 = Excitation energy (eV); Row 2 = Excited state; Row 3+ = Occ. --> Virt.												
Molecule	Excitation	Type	Reference	HF	B3LYP	ωB97	ωB97X	ωB97X-D	LRC-ωPBEh	M06	M06-2X	M06-HF
Dipeptide	n ₁ --> π ₂ *	CT	8.07	11.7552 (57)	6.3079 (10)	9.1056 (26)	8.6856 (25)	7.8785 (18)	7.7208 (20)	6.6315 (12)	8.2583 (23)	10.3411 (51)
				33 --> 4	35 --> 1	34 --> 1	34 --> 1	35 --> 1	35 --> 1	35 --> 1	34 --> 2	33 --> 3
				8.7133 (11)	6.1524 (8)	7.5003 (8)	7.3359 (8)	6.9793 (8)	6.8912 (8)	6.4555 (9)	7.1420 (9)	8.5555 (18)
Acene (n=1)	1B _{2u}	L	4.88	6.9420 (6)	5.7721 (6)	6.0249 (6)	5.9820 (6)	5.9254 (6)	5.8972 (6)	5.7970 (6)	5.7282 (6)	5.1835 (6)
				32 --> 4	32 --> 1	32 --> 1	32 --> 1	32 --> 1	32 --> 1	33 --> 1	32 --> 2	32 --> 3
				6.7150 (5)	5.5486 (5)	5.7942 (5)	5.7497 (5)	5.6917 (5)	5.6573 (5)	5.5588 (5)	5.4942 (5)	4.9521 (3)
Acene (n=2)	1B _{3u}	L	3.89	5.1037 (5)	4.3791 (5)	4.8747 (7)	4.8127 (7)	4.6891 (7)	4.6940 (7)	4.3248 (6)	4.7410 (6)	5.0424 (5)
				34 --> 1	34 --> 1	34 --> 1	34 --> 1	34 --> 1	34 --> 1	34 --> 1	34 --> 1	34 --> 1
				5.2512 (6)	4.4714 (7)	4.7046 (6)	4.6783 (6)	4.6283 (6)	4.6261 (6)	4.3986 (7)	4.6779 (5)	4.9082 (4)
PP	3 ¹ A ₁	CT	5.94	7.6494 (17)	4.6429 (6)	6.8482 (14)	6.5849 (13)	6.0233 (11)	5.9839 (11)	5.0429 (11)	5.8507 (11)	6.9874 (11)
				37 --> 2	38 --> 2	37 --> 2	37 --> 2	38 --> 2	38 --> 2	38 --> 2	38 --> 2	37 --> 2
				6.1366 (10)	4.5803 (9)	5.6887 (9)	5.5649 (9)	5.3128 (9)	5.2958 (9)	4.6660 (9)	5.2831 (8)	5.7978 (9)
PA oligomer (n=2)	1 ¹ B _u	L	5.92	5.6837 (7)	4.9657 (10)	5.3195 (8)	5.2690 (8)	5.1604 (7)	5.1645 (7)	4.7511 (6)	5.1622 (6)	5.4038 (6)
				38 --> 1	37 --> 1	38 --> 1	38 --> 1	37 --> 1	37 --> 1	37 --> 1	37 --> 1	38 --> 1
				5.7857 (8)	4.7647 (8)	5.2088 (7)	5.1669 (5)	5.0801 (5)	5.0752 (7)	4.7846 (5)	5.1006 (5)	5.3886 (5)
H ₂ CO (Singlet)	1A ₂	R	9.22	10.6640 (22)	8.2191 (23)	9.3477 (24)	9.2210 (25)	8.6771 (22)	8.5469 (22)	7.7581 (23)	9.1463 (26)	10.2988 (27)
				8 --> 9	8 --> 11	8 --> 10	8 --> 10	8 --> 10	8 --> 10	8 --> 10	8 --> 10	8 --> 10
				9.7586 (14)	7.4097 (10)	8.3862 (12)	8.2945 (12)	7.7878 (11)	7.6251 (11)	6.7537 (11)	8.1672 (12)	8.8655 (13)
HCl	1Π	CT	8.23	8.5410 (3,4)	7.6593 (3,4)	8.2049 (3,4)	8.0952 (3,4)	8.0106 (3,4)	7.9434 (3,4)	7.5910 (3,4)	7.7967 (3,4)	7.4933 (3,4)
				8 --> 1	8 --> 1	8 --> 1	8 --> 1	8 --> 1	8 --> 1	8 --> 1	8 --> 1	8 --> 1
				8.5410 (3,4)	7.6593 (3,4)	8.2049 (3,4)	8.0952 (3,4)	8.0106 (3,4)	7.9434 (3,4)	7.5910 (3,4)	7.7967 (3,4)	7.4933 (3,4)