Tables

TABLES

TABLE I. Excitation energies (ω_X in eV) and oscillator strengths (f_X) for excitations from the ground state, and excitation energies (ω_A in eV) and oscillator strengths (f_A) for excitations from the first excited singlet state for CO. t-aug-cc-pTVZ basis set, $R = 2.1322$ a.u. (exp from Ref [32]).

state	method	ω_X	f_X	ω_A	f_A
$A^1\Pi$	SCF	8.77	0.0848		
	CAS(g)	8.69	0.0841		
	CAS(x)	9.71			
	CCS	9.06	0.0953		
	CC2	8.67	0.0830		
	CCSD	8.62	0.0824		
	CCSDR(3)	8.55	0.0817		
	CC3	8.52	0.0814		
	exp	8.07 [a]			
$B^1\Sigma$	SCF	11.87	0.0580	3.10	0.0227
	CAS(g)	11.47	0.0446	2.78	0.0257
	CAS(x)			2.69	0.0008
	CCS	11.90	0.0558	2.84	0.0244
	CC2	10.82	0.0069	2.15	0.0211
	CCSD	10.96	0.0099	2.34	0.0240
	CCSDR(3)	10.72	0.0095	2.18	0.0223
	CC3	10.67	0.0095	2.16	0.0222
	exp	10.78 [a]			
$C^1\Sigma$	SCF	12.54	0.0810	3.77	0.0004
	CAS(g)	12.09	0.1029	3.40	0.0010

	CAS(x)			3.61	0.0424
	CCS	12.55	0.0863	3.49	0.0002
	CC2	11.39	0.1257	2.72	0.0092
	CCSD	11.56	0.1325	2.94	0.0081
	CCSDR(3)	11.45	0.1297	2.78	0.0077
	CC3	11.28	0.1292	2.77	0.0076
	exp	11.40 [a]			
$E^1\Pi$	SCF	12.58	0.0371	3.81	0.0170
	CAS(g)	12.18	0.0406	3.45	0.0152
	CAS(x)			4.34	0.0061
	CCS	12.59	0.0358	3.53	0.0156
	CC2	11.51	0.0353	2.84	0.0108
	CCSD	11.70	0.0362	3.08	0.0105
	CCSDR(3)	11.45	0.0355	2.91	0.0099
	CC3	11.41	0.0353	2.89	0.0098
	exp	11.52[a]			
$F^1\Sigma$	SCF	13.52	0.0427	4.75	0.0068
	CAS(g)	13.11	0.0284	4.37	0.0131
	CAS(x)			4.43	0.0076
	CCS	13.54	0.0208	4.49	0.0083
	CC2	12.39	0.0038	3.72	0.0160
	CCSD	12.63	0.0039	3.94	0.0090
	CCSDR(3)	12.31	0.0038	3.76	0.0086
	CC3	12.26	0.0038	3.74	0.0086
	exp	12.37[a]			
$G^1\Pi$	SCF	13.63	0.0023	4.85	0.0013
	CAS(g)	13.20	0.0192	4.47	0.0033

CAS(x)			5.35	0.0037
CCS	13.63	0.0021	4.57	0.0016
CC2	12.46	0.000002	3.79	0.0057
CCSD	12.71	0.0001	4.08	0.0057
CCSDR(3)	12.45	0.0001	3.90	0.0054
CC3	12.40	0.0001	3.88	0.0054

[a] T_e from Ref. [32]

TABLE II. Excitation energies (ω_X in eV) and oscillator strengths (f_X) for excitations from the ground state, and excitation energies (ω_A in eV) and oscillator strengths (f_A) for excitations from the first excited singlet state for formaldehyde. Sadlejs basis set. SCF/Sadlej geometry.

state	method	ω_X	f_X	ω_A	f_A
1^1A_2	SCF	4.54			
$(n \rightarrow \pi^*)$	CAS(g)	4.51			
	CAS(x)	5.18			
	CCS	4.70			
	CC2	4.23			
	CCSD	4.16			
	CCSDR(3)	4.15			
	CC3	4.16			
	exp	3.495 [a], 3.94 [b]			
1^1B_2	SCF	8.49	0.0300	3.95	0.0411
$(n \rightarrow 3s)$	CAS(g)	7.66	0.0194	3.15	0.0179
	CAS(x)			4.07	0.0160
	CCS	8.50	0.0306	3.80	0.0356
	CC2	6.40	0.0262	2.17	0.0223
	CCSD	6.99	0.0222	2.83	0.0209
	CCSDR(3)	7.00	0.0222	2.85	0.0210
	CC3	7.01	0.0222	2.86	0.0210
	exp	7.089[a]			
2^1B_2	SCF	9.36	0.0422	4.82	0.00004
$(n \rightarrow 3p_z)$	CAS(g)	8.60	0.0490	4.08	0.0048
	CAS(x)			5.23	0.0001
	CCS	9.37	0.0429	4.66	0.0002
	CC2	7.45	0.0317	3.22	0.0020

	CCSD	7.93	0.0395	3.77	0.0033
	CCSDR(3)	7.95	0.0385	3.80	0.0033
	CC3	7.97	0.0396	3.81	0.0033
	exp	8.115 [a]			
2^1A_2	SCF	9.96		5.42	0.0121
$(n \rightarrow 3p_x)$	CAS(g)	9.00		4.49	0.0196
	CAS(x)			5.80	0.0167
	CCS	9.96		5.26	0.0150
	CC2	7.92		3.70	0.0240
	CCSD	8.43		4.27	0.0210
	CCSDR(3)	8.47		4.32	0.0215
	CC3	8.49		4.33	0.0215
	exp	8.374 [b]			
1^1B_1	SCF	10.02	0.00008	5.49	0.0001
$(\sigma \rightarrow \pi^*)$	CAS(g)	10.08	0.0016	5.57	0.0005
	CAS(x)			5.54	0.0005
	CCS	10.25	0.00006	5.55	0.0003
	CC2	9.29	0.0021	5.06	0.0362
	CCSD	9.68	0.0011	5.52	0.0003
	CCSDR(3)	9.62	0.0010	5.47	0.0003
	CC3	9.62	0.0010	5.47	0.0003

[a] 0-0 bands from Ref. [33]

[b] vertical excitation energies from Ref. [22] as cited in Ref. [23]

TABLE III. Excitation energies (ω_X in eV) and oscillator strengths (f_X) for excitations from the ground state, and excitation energies (ω_A in eV) and oscillator strengths (f_A) for excitations from the first excited singlet state for formamide. Basis set and geometry as in Ref. [17]

state	method	ω_X	f_X	ω_A	f_A
$1^1A''$	SCF	6.35	0.0007		
$(n \rightarrow \pi^*)$	CAS(g)	5.66	0.0004		
	CAS(x)	6.09			
	CCS	6.52	0.0008		
	CC2	5.70	0.0002		
	CCSD	5.66	0.0003		
	CCSDR(3)	5.63	0.0003		
	CC3	5.64	0.0003		
	Exp	5.6–5.8[a]	≈ 0.002[a]		
$2^1A'$	SCF	8.31	0.1678	1.96	0.00002
$(n \rightarrow 3s)$	CAS(g)	7.76	0.2240	2.10	0.000003
	CAS(x)			0.77	0.000003
	CCS	8.51	0.1247	1.99	0.0004
	CC2	6.17	0.0255	0.47	0.00004
	CCSD	6.84	0.0005	1.18	0.00002
	CCSDR(3)	6.67	0.0005	1.04	0.00002
	CC3	6.59	0.0005	0.95	0.00002
	Exp	6.2–7.0[b]			
$3^1A'$	SCF	8.89	0.0911	2.54	0.0089
$(n \rightarrow 3p_y)$	CAS(g)	8.76	0.0535	3.10	0.000007
	CAS(x)			2.59	0.0010
	CCS	8.95	0.1401	2.43	0.0093
	CC2	6.77	0.0759	1.07	0.0103

	CCSD	7.43	0.1314	1.77	0.0094
	CCSDR(3)	7.31	0.1292	1.68	0.0089
	CC3	7.27	0.1285	1.63	0.00860
$4^1A'$	SCF	9.21	0.0116	2.86	0.00009
$(\pi \rightarrow \pi^*)$	CAS(g)	9.05	0.0051	3.38	0.0019
	CAS(x)			3.24	0.0109
	CCS	9.24	0.0054	2.72	0.00003
	CC2	7.23	0.0232	1.53	0.00002
	CCSD	7.64	0.2183	1.98	0.0026
	CCSDR(3)	7.52	0.2149	1.89	0.0025
	CC3	7.50	0.2145	1.86	0.0025
	Exp	≈ 7.4[d]			
$2^1A''$	SCF	7.68	0.0213	1.33	0.00004
$(\pi \rightarrow 3s)$	CAS(g)	7.64	0.0220	1.87	0.0002
	CAS(x)			3.76	0.0147
	CCS	7.07	0.0216	1.19	0.000008
	CC2	6.58	0.0227	0.88	0.000009
	CCSD	6.74	0.0221	1.08	0.000005
	CCSDR(3)	6.65	0.0219	1.02	0.000005
	CC3	6.64	0.0218	1.00	0.000005
$3^1A''$	SCF	8.57	0.000001	2.22	0.0008
$(\pi \rightarrow 3p_y)$	CAS(g)	8.27	0.00009	2.61	0.00005
	CAS(x)			4.40	0.0021
	CCS	8.59	0.000001	2.07	0.00006
	CC2	7.32	0.0081	1.62	0.0154
	CCSD	7.58	0.0002	1.92	0.00007
	CCSDR(3)	7.49	0.0002	1.86	0.00007

	CC3	7.49	0.0002	1.85	0.00007
$4^1A''$	SCF	9.18	0.0159	2.83	0.00000007
$(n \rightarrow 3p_z)$	CAS(g)	8.89	0.0110	3.22	0.0001
	CAS(x)			5.34	0.0004
	CCS	9.20	0.0162	2.68	0.000051
	CC2	7.39	0.00007	1.69	0.000002
	CCSD	8.02	0.0074	2.36	0.0152
	CCSDR(3)	7.91	0.0073	2.28	0.0147
	CC3	7.88	0.0072	2.24	0.0145
	Exp	7.7[d]			

[a]From Ref. [24]. Very weak peak.

[b]The energy span of the transition as given in Ref. [24]. Maximum absorption is around 6.3–6.4 eV

[c]Ref. [24]. Maximum absorption energy = 0-0 energy

[d]Ref. [24]. Maximum absorption energy = 0-0 energy

TABLE IV. Excitation energies (ω_X in eV) and oscillator strengths (f_X) for excitations from the ground state, and excitation energies (ω_A in eV) and oscillator strengths (f_A) for excitations from the first excited singlet state for sym-tetrazine. Basis set and geometry as in Ref. [18]

state	method	ω_X	f_X	ω_A	f_A
1^1B_{3u}	SCF	3.30	0.0083		
$(n(b_{3g}) \rightarrow 3d_{yz})$	CAS(g)	3.35	0.0140		
	CAS(x)				
	CCS	3.52	0.0100		
	CC2	2.42	0.0061		
	CCSD	2.66	0.0702		
	CCSDR(3)	2.56	0.0676		
	CC3	2.41	0.0637		
	exp	2.2–2.7 [a]			
1^1A_u	SCF	5.49			
$(n \rightarrow \pi^*)$	CAS(g)	5.08			
	CAS(x)				
	CCS	5.64			
	CC2	3.55			
	CCSD	3.95			
	CCSDR(3)	3.76			
	CC3	3.68			
1^1B_{1g}	SCF	5.92		2.62	0.048
$(n \rightarrow \pi^*)$	CAS(g)	5.55		2.20	0.039
	CAS(x)				
	CCS	6.13		2.61	0.0639
	CC2	5.06		2.64	0.1085
	CCSD	5.28		2.63	0.0757

	CCSDR(3)	5.11		2.55	0.0735
	CC3	4.85		2.44	0.0703
1^1B_{2u}	SCF	5.85	0.1350		
$(n \rightarrow \pi^*)$	CAS(g)	4.71	0.0526		
	CAS(x)				
	CCS	6.23	0.1340		
	CC2	5.29	0.0571		
	CCSD	5.34	0.0584		
	CCSDR(3)	5.28	0.0577		
	CC3	5.20	0.0569		
1^1B_{1u}	SCF	6.44	0.0009		
$(n \rightarrow 3p/\pi^*$ (mix))	CAS(g)	8.15	0.0349		
	CAS(x)				
	CCS	6.91	0.0027		
	CC2	6.85	0.0199		
	CCSD	7.40	0.0025		
	CCSDR(3)	7.34	0.0025		
	CC3	7.28	0.0024		
1^1B_{2g}	SCF	6.52		3.22	0.028
$(n \rightarrow \pi^*)$	CAS(g)	5.24		1.88	0.0065
	CAS(x)				
	CCS	6.76		3.24	0.0394
	CC2	5.67		3.25	0.0369
	CCSD	5.84		3.19	0.0263
	CCSDR(3)	5.65		3.09	0.0255
	CC3				
1^1B_{3g}	SCF	8.48			

$(n \rightarrow 3s)$	CAS(g)	7.95		
	CAS(x)			
	CCS	8.48		
	CC2	5.88		
	CCSD	6.54		
	CCSDR(3)	6.42		
	CC3	6.38		
2^1A_g	SCF	9.93	6.63	0.0032
$(n \rightarrow 3d)$	CAS(g)	8.68	5.33	0.0001
	CAS(x)			
	CCS	9.94	6.42	0.0026
	CC2	7.30	4.88	0.0035
	CCSD	8.08	5.42	0.0049
	CCSDR(3)	7.98	5.42	0.0049
	CC3	7.94	5.53	0.0050

[a]Maximum intensity peak = 0-0 transition energy for this transition. From Ref. [34] as cited in Ref. [18].

TABLE V. Excitation energies (ω_X in eV) for excitations from the ground state to the first excited singlet state for CO, formaldehyde, formamide and sym-tetrazine.

method	CO	formaldehyde	formamide	sym-tetrazine
SCF	8.77	4.54	6.35	3.30
CAS(g)	8.69	4.51	5.66	3.35
CAS(x)	9.71	5.18	6.09	
CCS	9.06	4.70	5.52	3.52
CC2	8.67	4.23	5.70	2.42
CCSD	8.62	4.16	5.66	2.66
CCSDR(3)	8.55	4.15	5.63	2.56
CC3	8.52	4.16	5.64	2.41
exp	8.07 [a]	3.395 [b], 3.94 [c]	5.6–5.8 [d]	2.2–2.7[e]

[a] T_e from Ref. [32]

[b] 0-0 bands from Ref. [33]

[c] vertical excitation energies from Ref. [22] as cited in Ref. [23]

[d]From Ref. [24]. Very weak peak.

[e]Maximum intensity peak = 0-0 transition energy for this transition. From Ref. [34] as cited in Ref. [18].

REFERENCES

[1] P.Å. Malmqvist and B. O. Roos Chem. Phys. Lett., **155**, 189 (1989).

[2] J. Olsen and P. Jørgensen, in Ed. Yarkony: *Modern electronic structure theory*, Part I. World scientific publishing Co. Singapore (1995).

[3] O. Christiansen, P. Jørgensen, and C. Hättig, Int. J. Quantum. Chem. **68**,1 (1998) and references therein.

[4] P. Norman, D. Jonsson, H. Ågren, P. Dahle, K. Ruud, T. Helgaker and H. Koch Chem. Phys. Lett. **253**, 1 (1996).

[5] D. Jonsson, P. Norman, K. Ruud, H. Ågren and T. Helgaker, J. Chem. Phys. **109**, 572 (1998).

[6] K. Ruud, D. Jonsson, P. Norman, H. Ågren, T. Saue, H. J. Aa. Jensen, P. Dahle, T. Helgaker and H. Koch J. Chem. Phys. **108**, 7973 (1998).

[7] O. Christiansen, H. Koch, and P. Jørgensen, Chem. Phys. Lett. **243**, 409 (1995).

[8] O. Christiansen, H. Koch, and P. Jørgensen, J. Chem. Phys. **103**, 7429 (1995).

[9] O. Christiansen, H. Koch, and P. Jørgensen, J. Chem. Phys. **105**, 1451 (1996).

[10] O. Christiansen, A. Halkier, H. Koch, P. Jørgensen, and T. Helgaker, J. Chem. Phys., **108** , 2801 (1998).

[11] D. Jonsson, P. Norman and H. Ågren, Chem. Phys. **224**, 201 (1997).

[12] O. Christiansen, H. Koch, P. Jørgensen, and J. Olsen, Chem. Phys. Letters **256**, 185 (1996)

[13] A.Sadlej, Coll. Czech. Chem. Commun. **53**, 1995 (1988).

[14] T.H. Dunning, J. Chem. Phys. **90**, 1007 (1989).

[15] R.A. Kendall, T.H. Dunning, and R.J. Harrison, J. Chem. Phys. **96**, 6769 (1992).

[16] D.E. Woon and T.H. Dunning, J. Chem. Phys. **100**, 2975 (1994).

[17] L. Serrano-Andres and M. Fulscher, J. Am. Chem. Soc. **118**, 12190 (1996).

[18] M. Rubio and B.O. Roos, Molecular Physics **96**, 603 (1999).

[19] "DALTON an electronic structure program, Release 1.0 (1997)", written by T.Helgaker, H. J. Aa. Jensen, P. Jørgensen, J. Olsen, K. Ruud, H. Ågren, T. Andersen, K. L. Bak, V. Bakken, O. Christiansen, P. Dahle, E. K. Dalskov, T. Enevoldsen, B. Fernandez, H. Heiberg, H. Hettema, D. Jonsson, S. Kirpekar, R. Kobayashi, H. Koch, K. V. Mikkelsen, P. Norman, M. J. Packer, T. Saue, P. R. Taylor, and O. Vahtras.

[20] H. Hettema, H.J.Aa. Jensen, P. Jørgensen and J. Olsen, J. Chem. Phys. **97**, 1174 (1992).

[21] O. Christiansen, H. Koch, A. Halkier, P. Jørgensen, T. Helgaker, and A. Sanchez de Meras, J. Chem. Phys. **105**, 6921 (1996).

[22] S. Taylor, D. G. Wilden and J. Comer, Chem. Phys. **70**, 291 (1982).

[23] D. J. Clouthier and D. A. Ramsay, Annu. Rev. Phys. Chem. **34**, 31 (1983).

[24] J.M. Gingell, N.J. Mason, H. Zhao, I.C. Walker, and M.R.F. Siggel, Chem. Phys. **220**, 191 (1997).

[25] J.F. Stanton and J. Gauss, J. Chem. Phys. **104**, 9859 (1996).

[26] A.C. Scheiner and H.F.Schaefer, J. Chem. Phys. **87**, 3539 (1987).

[27] K. K. Innes, J. Mol. Spectrosc. **129**, 140 (1988).

[28] P. Norman, D. Jonsson and H. Ågren, Chem. Phys. Lett. **268**, 337 (1997).

[29] D. Jonsson, P. Norman, Y. Luo, and H. Ågren, J. Chem. Phys. **105**, 581 (1996).

[30] H. Ågren, A. Flores-Riveros, and H.J. Aa. Jensen, Physica Scripta, **40**, 745, (1989).

[31] Y. Luo, P. Norman, P. Macak, and H. Ågren. J. Phys. Chem. **104**, 4718 (2000).

[32] G. Herzberg and K. P. Huber, *Molecular spectra and molecular structure* , Van Nostrand, New York (1979).

[33] C. R. Lessard and D. C. Moule, J. Chem. Phys. **66**, 3906 (1977).

[34] S. F. Mason, J. Chem. Soc. **1263**, (1959).