Erratum

FTIR Spectroscopic and Theoretical Study of the Photochemistry of Matrix-isolated Coumarin

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In the most recent issue of *Photochemistry and Photobiology*, 2007, **83**(5), 1237–1253, an error in Table 2 was published.

The corrected Table 2 is shown:

Table 2. Frequencies (cm^{-1}) and intensities (km mol^{-1}) of monomeric coumarin theoretically calculated at the B3LYP/6-311 + +G(d,p) and MP2/6-31G(d,p) levels compared to the observed infrared spectrum of coumarin isolated in an argon matrix at 10 K*.

Approximate description†	Sym.	Calculated DFT(B3LYP)/ 6-311 + +G(d,p) Freq.‡	Int.	Calculated MP2/6-31G(d,p) Freq.§	Int.	Observed spectrum Ar (10 K) Freq.	Int.‖
ν(C3–H)	A′	3099	0.3	3100	0.5	–	
ν(C7–H)	A′	3088	3.2	3087	4.1	3096	1.0
ν(C9–H)	A′	3079	11.0	3079	10.6	3085,3079	1.5
ν(C8–H)	A′	3065	7.0	3064	5.5	3059	1.0
ν(C10–H)	A′	3055	5.2	3050	0.9	3053	1.1
ν(C4–H)	A′	3051	4.1	3052	11.0	3043	0.7
ν(C=O)	A′	1772	718.0	1757	422.3	1776,1774,1772,1767,1762, 1759,1752,1748,1747	456.6
ν(C3=C4)	A′	1633	65.9	1628	24.8	1635,1632,1631,1630	45.0
ν(C10–C9)	A′	1616	60.7	1608	25.7	1617,1613,1612,1610	54.1
ν(C8–C7)	A′	1568	39.3	1566	6.3	1572,1571	12.7
δ(C–H) *ph*	A′	1489	5.2	1484	8.4	1492	3.2
ν(C7–C6)	A′	1453	23.4	1445	31.6	1459,1458,1455	25.8
δ(C–H) *py*	A′	1400	10.1	1425	11.6	1399	9.8
ν(C5–C6)/ δ(C–H) *ph*	A′	1336	2.7	1390	12.8	1329,1327	1.9
δ(C–H) *ph*/ ν(C5–C6)	A′	1273	20.7	1258	27.3	1278,1276,1275	13.2
ν(C6–O)	A′	1255	28.6	1242	14.0	1263,1262,1260,1259	17.6
ν(C4–C5)	A′	1225	13.1	1224	2.2	1233,1232,1228,1226,1225	13.8
δ(C–H) *py*/ ν(C2–C3)	A′	1169	25.6	1174	99.5	1202,1197,11961194,1181,1178	69.2
δ(C–H) *ph*	A′	1156	0.9	1151	0.9	1156,1153	1.2
δ(C–H) *ph*	A′	1118	20.5	1111	47.5	1134,1132,1129,1128,1123,1119,1118	32.6
ν(C2–C3)/ δ(C–H) *py*	A′	1075	99.8	1088	49.2	1106,1102,1098,1097	56.1
ν(C9–8)	A′	1030	2.2	1021	1.3	1031,1030	1.0
γ(C–H) *py*	A″	983	0.5	964	0.5	984,982	0.2
γ(C–H) *ph*	A″	969	0.2	917	0.3	–	
γ(C−H) *ph*	A″	948	3.2	903	0.5	945,944,942,940	3.4
ν(O−C2)/ δ ring *ph*	A′	922	28.8	911	23.5	929,927,926	19.8
δ ring *ph*/ ν(O–C2)	A′	875	43.3	949	41.5	888,886	21.0
γ(C–H) *ph*	A″	863	3.1	843	0.6	866,865,864	2.3
γ(C–H) *py*	A″	830	59.1	827	61.0	832,829,828,827	52.2
ν(C10–C5)	A′	761	2.5	785	2.6 ⎫	765,763,762,761,759,753	56.2
γ(C–H) *ph*	A″	761	46.8	763	46.0 ⎭		
τ ring *py*¶	A″	740	15.9				
δ ring *ph*	A′	731	2.6	754	1.7	726,725	1.1
γ(C=O)	A″	678	0.5	669	4.2	680	0.2
δ ring *py*	A′	614	8.3	626	9.7	610	7.3
τ ring *py*	A″	538	0.2	503	0.0	–	
δ ring *py*	A′	530	6.7	542	3.9	527,526	2.0
δ(C=O)	A′	489	5.4	497	3.9	490,486(?)	0.6
τ Butterfly	A″	454	5.2	435	1.3	459,452	4.6
δ ring *ph*	A′	445	1.5	456	0.8	446	0.3

Table 2. (Continued)

Approximate description†	Sym.	Calculated DFT(B3LYP)/ 6-311 + +G(d,p)		Calculated MP2/6-31G(d,p)		Observed spectrum Ar (10 K)	
		Freq.‡	Int.	Freq.§	Int.	Freq.	Int.‖
τ ring *py*¶	A″			355	0.4		
τ ring *ph*	A″	369	0.1	327	0.1		
δ ring *py*	A′	304	0.8	308	1.0	Not investigated	
τ ring *py*	A″	253	0.5	243	0.3		
τ ring *ph*	A″	154	4.6	154	4.5		
τ ring *ph*	A″	93	1.4	93	1.2		

*See Table S1 for definition of symmetry coordinates and Tables S2 and S3 for PEDs calculated using the DFT and MP2 force constants and geometries, respectively. †Approximate description is known to be an oversimplification of the vibrations description, where their description in terms of a single, most significant symmetry coordinate was attempted. The detailed description is given in the PED form (Tables S2 and S3). *v*, bond stretching; δ, bending; γ, rocking; τ, torsion; *ph*, phenyl ring; *py*, pyrone ring. Wherever two approximate descriptions are given, separated by a slash (/) symbol, the left one corresponds to the approximate description extracted from the PEDs calculated at the DFT(B3LYP)/6-311 + +G(d,p) level and the right one to that obtained based on the MP2/6-31G(d,p) calculations. ‡Theoretical positions of absorption bands were scaled by a factor 0.964 in the 4000–2500 cm^{-1} region; 0.982 in the 2500–1000 cm^{-1} region and 0.989 in the region below 1000 cm^{-1}. §Theoretical positions of absorption bands were scaled by a factor of 0.938 in the 4000–2500 cm^{-1} region; 0.956 in the 2500–1000 cm^{-1} region and 1.014 in the region below 1000 cm^{-1}. ‖Observed intensities (Int_{exp}) correspond to band integral absorbances (A) normalized by the theoretical intensities (Int_{calc}) at MP2/6-31G(d,p) level, according to the formula $Int_{exp}^{(i)} = A^{(i)} \Sigma Int_{calc} / \Sigma A$, where the sums extend to all theoretical bands which have an experimentally observed counterpart. ¶In the low frequency region the torsional vibrations of the pyrone ring were predicted in a substantially different way by the DFT(B3LYP)/6-311 + +G(d,p) and MP2/6-31G(d,p) methods.