

Vibrationally-resolved spectroscopic studies of electronically excited states of 1,8-naphthalic anhydride and 1,8-naphthalimide: a delicate interplay between one  $\pi\pi^*$  and two  $n\pi^*$  states

## Supporting Information

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Table SII: Excitation energies (E) and normalized intensities (I) of bands observed in the 30260-31400  $\text{cm}^{-1}$  region of 1,8-naphthalic anhydride (NA) and 29910-30910  $\text{cm}^{-1}$  region of 1,8-naphthalimide (NI)

1,8-naphthalic anhydride			1,8-naphthalimide		
E ( $\text{cm}^{-1}$ )	E* ( $\text{cm}^{-1}$ )	I	E ( $\text{cm}^{-1}$ )	E* ( $\text{cm}^{-1}$ )	I
30268.2	0	1	29919.5	-143	0.05
30460.1	191.9	0.12	29925.8	-136.7	0.04
30478.7	210.5	0.2	29934.7	-127.8	0.05
30489.8	221.6	0.13	29938.3	-124.2	0.05
30521.5	253.3	0.87	29953.5	-109	0.07
30579.4	311.2	0.13	29960.7	-101.8	0.06
30613.1	344.9	0.33	30015.6	-46.9	0.18
30622.4	354.2	0.42	30062.5	0	1
30636.5	368.3	0.68	30067	4.5	0.16
30705.1	436.9	0.92	30073.4	10.9	0.08
30713.7	445.5	0.3	30178.6	116.1	0.08
30801.6	533.4	0.55	30203.2	140.7	0.32
30832	563.8	0.19	30227	164.5	0.26
30843.5	575.3	0.14	30237.9	175.4	0.18
30847.3	579.1	0.34	30244.3	181.8	0.15
30860.6	592.4	0.4	30249.8	187.3	0.18
30865.3	597.1	0.23	30254.4	191.9	0.3
30879.6	611.4	0.24	30260.8	198.3	0.39
30887.3	619.1	0.18	30267.2	204.7	0.19
30918.8	650.6	0.14	30270.9	208.4	0.16
30961.9	693.7	0.13	30275.5	213	0.16
30969.5	701.3	0.29	30281	218.5	0.17
30981.1	712.9	0.27	30283.7	221.2	0.16
30991.6	723.4	0.23	30287.4	224.9	0.17
30995.5	727.3	0.13	30292.9	230.4	0.14
31006	737.8	0.11	30294.7	232.2	0.13
31065.7	797.5	0.14	30299.3	236.8	0.07
31069.6	801.4	0.35	30304.84	242.34	0.61
31076.4	808.2	0.14	30335.2	272.7	0.06
31090.9	822.7	0.15	30354.5	292	0.06
31151.9	883.7	0.17	30367.4	304.9	0.15
31166.5	898.3	0.37	30370.2	307.7	0.19

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<b>E (cm<sup>-1</sup>)</b>	<b>E* (cm<sup>-1</sup>)</b>	<b>I</b>	<b>E (cm<sup>-1</sup>)</b>	<b>E* (cm<sup>-1</sup>)</b>	<b>I</b>
31170.3	902.1	0.3	30372.9	310.4	0.16
31172.3	904.1	0.29	30378.5	316	0.22
31176.1	907.9	0.29	30385	322.5	0.45
31181	912.8	0.24	30394.2	331.7	0.17
31183.9	915.7	0.17	30397.1	334.6	0.08
31186.8	918.6	0.23	30415.4	352.9	0.08
31189.8	921.6	0.14	30446	383.5	0.08
31197.5	929.3	0.13	30453.4	390.9	0.13
31216	947.8	0.1	30455.3	392.8	0.13
31224.8	956.6	0.1	30459.9	397.4	0.12
31248.2	980	0.17	30461.8	399.3	0.18
31251.2	983	0.13	30465.5	403	0.15
31259	990.8	0.35	30468.3	405.8	0.11
31271.7	1003.5	0.1	30862.3	799.8	0.07
31291.2	1023	0.15	30567.9	505.4	0.06
31295.2	1027	0.15	30576.3	513.8	0.05
31300.1	1031.9	0.25	30619.4	556.9	0.17
31341.3	1073.1	0.24	30658.8	596.3	0.08
31346.2	1078	0.13	30692.7	630.2	0.08
31355	1086.8	0.13	30763.5	701	0.09
31374.7	1106.5	0.13	30775.8	713.3	0.1
31380.6	1112.4	0.13	30785.3	722.8	0.12
			30819.5	757	0.12
			30827.1	764.6	0.13
			30830.9	768.4	0.15
			30837.5	775	0.1
			30860.4	797.9	0.09
			30873.7	811.2	0.08
			30887	824.5	0.14
			30890.9	828.4	0.12
			30895.6	833.1	0.1
			30909	846.5	0.1

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\* relative to 0-0 transition

Table SI2: Calculated harmonic frequencies of 1,8-naphthalic anhydride and 1,8-naphthalimide in  $2^1A_1(\pi\pi^*)$  state. Frequencies have been scaled with a factor of 0.960

<u>1,8-naphthalic anhydride</u>			<u>1,8-naphthalimide</u>	
<u>symm.</u>	<u>label</u>	<u>freq., cm<sup>-1</sup></u>	<u>label</u>	<u>freq.,cm<sup>-1</sup></u>
a <sub>1</sub>	1	3140	1	3476
	2	3114	2	3138
	3	3098	3	3111
	4	1773	4	3096
	5	1609	5	1707
	6	1480	6	1608
	7	1446	7	1479
	8	1384	8	1457
	9	1382	9	1384
	10	1310	10	1380
	11	1168	11	1347
	12	1110	12	1186
	13	1059	13	1141
	14	926	14	1061
	15	788	15	933
	16	638	16	788
	17	558	17	669
	18	434	18	560
	19	421	19	445
	20	346	20	421
			21	341
a <sub>2</sub>	1	946	1	946
	2	835	2	837
	3	743	3	751
	4	693	4	699
	5	507	5	513
	6	343	6	353
	7	201	7	208
	8	66	8	78
b <sub>1</sub>	1	947	1	948

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<b>symm.</b>	<b>label</b>	<b>freq., cm<sup>-1</sup></b>	<b>label</b>	<b>freq.,cm<sup>-1</sup></b>
	2	878	2	877
	3	761	3	767
	4	693	4	720
	5	674	5	694
	6	471	6	659
	7	427	7	470
	8	195	8	430
	9	143	9	198
	10	132	10	151
			11	132
b <sub>2</sub>	1	3139	1	3137
	2	3113	2	3110
	3	3096	3	3093
	4	1724	4	1698
	5	1552	5	1553
	6	1451	6	1440
	7	1405	7	1404
	8	1390	8	1392
	9	1226	9	1356
	10	1159	10	1228
	11	1139	11	1184
	12	1057	12	1130
	13	1002	13	1112
	14	980	14	1050
	15	784	15	992
	16	655	16	757
	17	509	17	642
	18	384	18	506
	19	273	19	374
			20	272