Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Online Supplementary material for: Determination of the Geometry Change of 5-Cyanoindole upon Electronic Excitation from a Combined Franck-Condon/Rotational Constants Fit.

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The online supporting material contains:

- Figure S1 The fluorescence emission spectra through the vibronic bands at 666 cm^{-1}, 876 cm^{-1}, and 884 cm^{-1}.
- Table S1 SCS-CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates.
- Table S2 SCS-CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates.
- Table S3 Experimental intensities of the assigned bands in the DF and LIF spectra.
- Table S4 Complete Duschinsky matrix for the S_0 and S_1 modes of 5CI

Table S1: SCS-CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 5CI (in bohr).

c	2.35019781	-3.46398276	-0.06583061
c	1.28135652	-0.97281537	-0.00578832
c	-1.38961411	-1.25884087	-0.06860637
n	-1.89043978	-3.80593228	-0.16184733
c	0.36301331	-5.13025296	-0.16013315
c	2.31302511	1.46736094	0.09439528
c	0.67241128	3.52912870	0.12867474
c	-1.98699674	3.20244899	0.06483292
c	-3.04346320	0.80888173	-0.03428126
c	1.68504998	6.04595455	0.23055902
n	2.50559442	8.11020028	0.31366763
h	4.32368942	-3.96057592	-0.04256695
h	0.36148410	-7.16517968	-0.22675658
h	-3.61968003	-4.58790024	-0.22239344
h	4.33593391	1.76399170	0.14448228
h	-5.07329575	0.56211543	-0.08298895
h	-3.18826627	4.85539776	0.09458110

Table S2: SCS-CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 5CI (in bohr).

c	2.34807092	-3.45121350	-0.06567041
c	1.31745932	-0.98607006	-0.00698208
c	-1.42925839	-1.27098536	-0.07067684
n	-1.90275426	-3.83626947	-0.16247871
c	0.34811237	-5.16343948	-0.16031102
c	2.41402094	1.45822464	0.09393837
c	0.70538740	3.58187038	0.12996315
c	-2.00778801	3.23347115	0.06409216
c	-3.10968351	0.78973714	-0.03755976
c	1.67494416	6.07294292	0.23293712
n	2.48621201	8.15247905	0.31986988
h	4.32112387	-3.95620480	-0.04261124
h	0.36191796	-7.19766887	-0.22525079
h	-3.62911603	-4.62778158	-0.22186540
h	4.43380807	1.74901566	0.14363946
h	-5.13799148	0.55595816	-0.08572679
h	-3.19446532	4.89593403	0.09469290

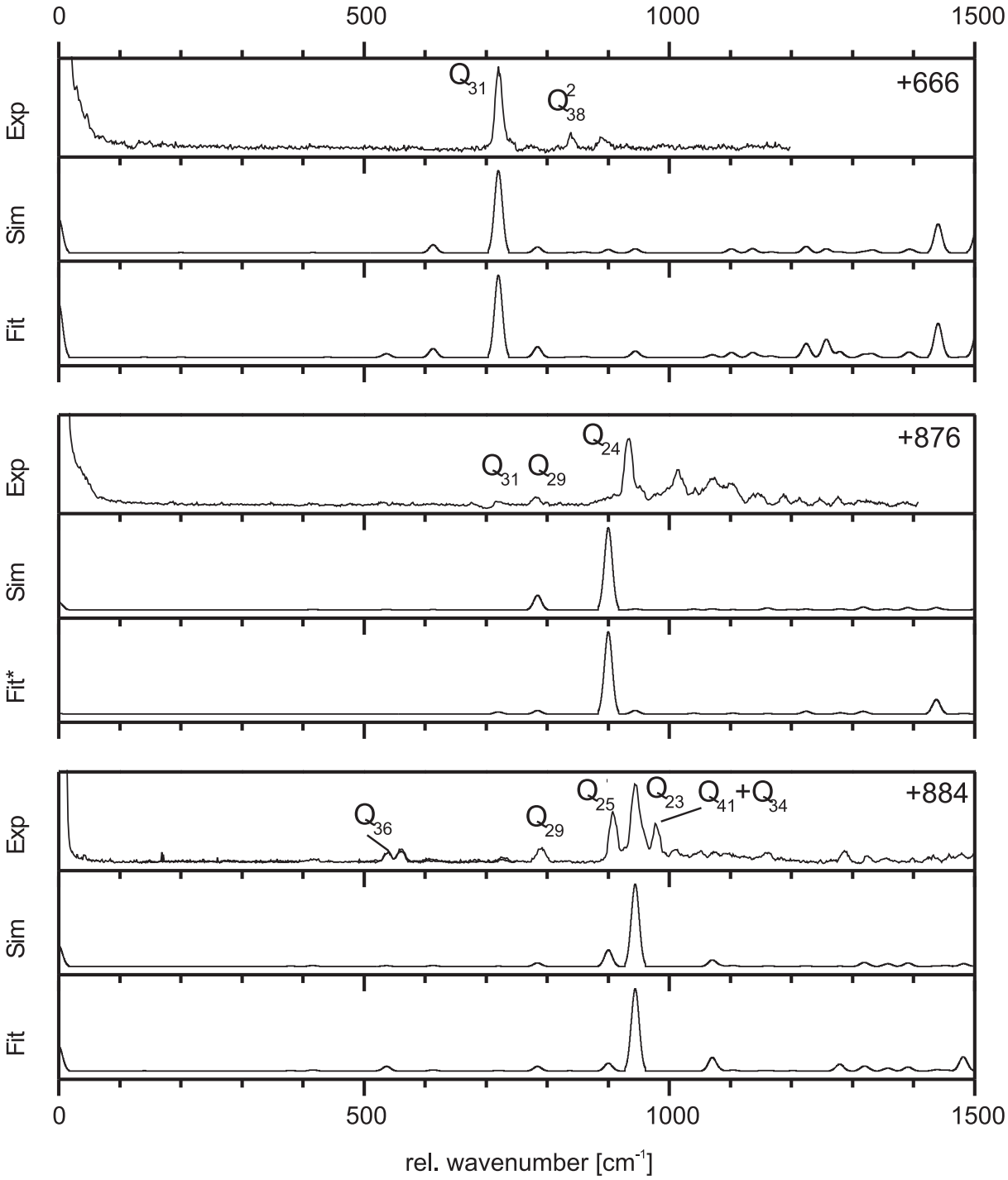

Figure S1: Dispersed fluorescence spectra of 5CI obtained via pumping the vibronic bands at 666 cm^{-1}, 876 cm^{-1}, and 884 cm^{-1}. Within each block, the first trace gives the experimental spectrum, the second trace a FC simulation using the *ab initio* values, and the third trace the FC fit. See text for details.

Table S4: Complete Duschinsky matrix for the S_0 and S_1 modes of 5CI, calculated from the CC2/cc-pVTZ structures and Hessians.

Nr.	S_0/S_1	77.2	134.7	172.1	224.3	308.7	334.4
Q_{45}	105.2	-0.99266	-0.00150	-0.02392	0.00706	0.09688	0.01757
Q_{44}	139.2	0.00148	-0.99950	0.00087	0.00034	-0.00001	-0.00026
Q_{43}	225.7	-0.02643	0.00080	0.99049	-0.09676	0.00395	-0.07872
Q_{42}	263.9	0.01518	0.00044	0.10437	0.98138	0.01701	0.03902
Q_{41}	379.1	-0.00030	0.01045	-0.00057	0.00047	0.00169	-0.02373
Q_{40}	400.2	0.00066	-0.00018	-0.06837	0.01797	0.06434	-0.97164
Q_{39}	417.1	0.00154	0.00263	-0.00022	-0.00039	0.00532	0.01346
Q_{38}	421.3	-0.08688	-0.00007	0.00434	-0.00462	-0.97853	-0.03145
Q_{37}	481.7	-0.07074	-0.00006	-0.02420	0.15862	-0.13447	-0.15762
Q_{36}	532.2	-0.00005	0.02166	-0.00037	0.00020	0.00083	-0.0034
Q_{35}	606.1	0.00490	0.00008	0.03538	-0.03401	0.04596	0.10667
Q_{34}	613.8	-0.00009	0.00841	-0.00047	0.00049	0.00042	-0.0028
Q_{33}	633.2	-0.01883	-0.00001	-0.00179	-0.00982	-0.05274	-0.0894
Q_{32}	722.0	-0.02359	-0.00002	0.01999	-0.01597	-0.01152	0.0268
Q_{31}	729.2	-0.00018	-0.00614	0.00015	0.00046	-0.00015	0.0026
Q_{30}	758.4	-0.00592	-0.00003	0.00458	-0.01007	0.03019	0.0152
Q_{29}	788.2	-0.00030	0.00104	0.00019	-0.00031	0.00021	-0.00101
Q_{28}	812.4	-0.00041	0.00001	0.01241	0.00374	0.06255	-0.02543
Q_{27}	853.3	0.00371	0.00000	-0.00917	0.00909	-0.00159	-0.01360
Q_{26}	896.8	-0.00323	-0.00000	0.01519	0.01464	-0.02465	-0.01002
Q_{25}	900.7	-0.00018	0.00325	-0.00031	-0.00002	0.00006	-0.00102
Q_{24}	934.2	-0.00473	-0.00001	-0.00067	-0.00034	-0.00712	-0.00276
Q_{23}	946.4	0.00021	0.00018	0.00002	-0.00006	0.00010	-0.00038
Q_{22}	1087.9	0.00018	0.00185	0.00007	0.00020	0.00005	-0.00084
Q_{21}	1110.3	0.00001	0.00386	0.00002	-0.00002	0.00002	-0.00131
Q_{20}	1148.0	-0.00022	0.00317	-0.00020	0.00016	0.00033	-0.00073
Q_{19}	1159.6	-0.00004	-0.00070	0.00008	0.00012	-0.00018	0.00085
Q_{18}	1238.7	0.00011	0.01057	-0.00005	-0.00023	0.00026	-0.00204
Q_{17}	1269.9	0.00008	-0.00223	0.00014	0.00005	-0.00010	0.00043
Q_{16}	1303.8	-0.00020	0.00115	0.00008	-0.00018	0.00047	-0.00024
Q_{15}	1353.2	0.00014	-0.00548	-0.00002	0.00013	-0.00021	0.00056
Q_{14}	1390.2	0.00000	0.00391	0.00004	0.00017	-0.00020	-0.00034
Q_{13}	1457.3	-0.00004	0.00421	-0.00020	-0.00005	0.00027	-0.00090
Q_{12}	1487.0	-0.00006	-0.00562	0.00009	-0.00001	0.00017	0.00004
Q_{11}	1499.8	-0.00014	-0.00152	0.00004	0.00010	-0.00010	-0.00004
Q_{10}	1546.3	0.00006	-0.00623	-0.00003	0.00022	-0.00043	0.00172
Q_9	1611.8	-0.00004	0.00044	-0.00002	0.00010	-0.00010	0.00017
Q_8	1657.9	-0.00003	-0.00229	-0.00001	0.00012	-0.00002	0.00033
Q_7	2151.4	0.00028	0.00149	0.00006	-0.00042	-0.00036	0.00005
Q_6	3205.8	-0.00001	-0.00017	0.00001	0.00001	0.00000	0.00006
Q_5	3214.3	-0.00000	0.00032	-0.00000	0.00001	0.00001	0.00005
Q_4	3226.8	0.00000	0.00004	-0.00003	-0.00001	-0.00001	-0.00000
Q_3	3267.6	-0.00003	0.00039	0.00005	-0.00004	0.00002	0.00003
Q_2	3286.4	0.00003	-0.00010	-0.00003	0.00004	-0.00003	0.00006

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Q_1	3680.4	-0.00005	0.00007	0.00010	-0.00000	-0.00004	-0.00075
Nr.	S_0/S_1	341.0	374.2	394.9	474.3	508.0	551.4
Q_{45}	105.2	-0.00026	-0.06128	0.00081	-0.00007	0.01113	-0.01020
Q_{44}	139.2	0.01398	0.00010	0.00551	-0.02472	-0.00000	0.00000
Q_{43}	225.7	-0.00172	0.02642	0.00044	-0.00038	0.00370	-0.03497
Q_{42}	263.9	0.00083	-0.13653	0.00038	-0.00008	0.05311	0.04246
Q_{41}	379.1	0.86942	0.00264	0.46274	0.14228	0.00057	-0.00028
Q_{40}	400.2	-0.02677	-0.18969	0.00146	-0.00005	-0.05872	0.04510
Q_{39}	417.1	-0.43611	0.00177	0.88117	-0.10823	-0.00049	0.00002
Q_{38}	421.3	-0.00129	-0.16321	0.00594	-0.00152	-0.01027	0.02081
Q_{37}	481.7	-0.00593	0.87417	-0.00146	0.00089	-0.38955	-0.05844
Q_{36}	532.2	0.11645	0.00110	-0.00468	-0.88806	-0.00042	-0.00047
Q_{35}	606.1	0.00453	-0.19979	-0.00008	-0.00171	-0.61296	0.73633
Q_{34}	613.8	0.09311	0.00116	-0.02934	-0.35951	0.00227	-0.00348
Q_{33}	633.2	-0.00303	0.28664	-0.00044	-0.00065	0.66018	0.60591
Q_{32}	722.0	0.00002	0.14201	0.00019	0.00043	0.11123	0.22240
Q_{31}	729.2	-0.11977	-0.00075	0.06491	0.10972	-0.00054	0.00015
Q_{30}	758.4	-0.00009	0.05668	0.00006	0.00050	0.02384	0.13443
Q_{29}	788.2	0.00532	-0.00004	0.00847	-0.08215	-0.00027	0.00120
Q_{28}	812.4	-0.00112	0.03511	-0.00003	0.00055	0.01080	0.09656
Q_{27}	853.3	-0.00040	0.00546	-0.00010	0.00004	0.02277	-0.06657
Q_{26}	896.8	0.00018	-0.02528	-0.00020	0.00043	-0.11112	-0.01906
Q_{25}	900.7	0.01594	-0.00012	-0.01639	-0.02502	-0.00076	0.00107
Q_{24}	934.2	-0.00027	0.05214	0.00005	0.00005	0.06510	-0.00258
Q_{23}	946.4	0.00135	0.00026	0.01394	0.00009	0.00004	0.00013
Q_{22}	1087.9	0.03865	0.00023	-0.01131	-0.03067	0.00003	0.00015
Q_{21}	1110.3	0.03716	-0.00007	-0.02299	-0.04736	-0.00010	0.00003
Q_{20}	1148.0	0.02837	-0.00007	-0.00791	-0.05236	-0.00011	-0.00009
Q_{19}	1159.6	-0.02971	-0.00022	0.00548	0.00536	0.00000	-0.00007
Q_{18}	1238.7	0.07339	0.00019	-0.03544	-0.08862	-0.00012	0.00012
Q_{17}	1269.9	-0.01936	-0.00007	0.00554	0.02931	-0.00017	0.00025
Q_{16}	1303.8	0.00365	-0.00007	0.00243	-0.02524	-0.00011	0.00032
Q_{15}	1353.2	-0.03307	0.00003	0.00164	0.05856	0.00008	0.00032
Q_{14}	1390.2	0.02161	-0.00016	0.00225	-0.06290	-0.00023	0.00003
Q_{13}	1457.3	0.03797	0.00023	-0.01550	-0.04145	0.00002	0.00025
Q_{12}	1487.0	-0.00622	0.00005	0.01499	0.04772	-0.00001	0.00020
Q_{11}	1499.8	-0.01421	-0.00031	0.01592	0.00327	-0.00009	-0.00021
Q_{10}	1546.3	-0.04837	-0.00002	0.02948	0.05419	0.00009	0.00011
Q_9	1611.8	-0.00820	0.00001	0.00451	-0.00799	0.00011	-0.00020
Q_8	1657.9	-0.00308	-0.00000	0.00014	0.01647	-0.00005	0.00001
Q_7	2151.4	-0.00889	0.00068	0.00726	0.01151	-0.00077	-0.00015
Q_6	3205.8	-0.00050	0.00002	-0.00051	0.00144	0.00000	-0.00003
Q_5	3214.3	0.00000	0.00003	-0.00014	-0.00147	-0.00003	-0.00005
Q_4	3226.8	-0.00129	0.00001	0.00143	0.00230	0.00004	0.00002
Q_3	3267.6	0.00023	0.00002	-0.00068	-0.00094	0.00009	-0.00020
Q_2	3286.4	-0.00071	0.00003	0.00033	0.00075	-0.00003	0.00012
Q_1	3680.4	-0.00087	-0.00027	-0.00010	0.00062	-0.00012	0.00026

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Nr.	S_0/S_1	582.2	599.5	615.9	639.1	661.6	689.1
Q_{45}	105.2	-0.00006	-0.00759	0.01009	-0.00646	0.00033	-0.00281
Q_{44}	139.2	-0.00102	-0.00001	-0.00002	-0.00001	0.00492	0.00002
Q_{43}	225.7	-0.00024	0.00173	0.02305	-0.00691	0.00008	-0.00651
Q_{42}	263.9	0.00012	0.02219	-0.00289	0.01097	0.00062	0.00306
Q_{41}	379.1	0.04451	0.00025	0.00001	-0.00010	-0.06782	-0.00011
Q_{40}	400.2	-0.00028	0.04838	-0.00871	0.04488	0.00078	0.01010
Q_{39}	417.1	-0.07045	-0.00095	0.00023	0.00016	0.10861	0.00012
Q_{38}	421.3	-0.00045	0.04394	-0.04221	-0.04484	0.00067	-0.02183
Q_{37}	481.7	-0.00030	-0.01863	0.06511	-0.04285	0.00007	0.00210
Q_{36}	532.2	0.41610	-0.00044	0.00009	0.00004	-0.07598	-0.00020
Q_{35}	606.1	-0.00393	-0.02858	0.11579	-0.03160	-0.00072	-0.00086
Q_{34}	613.8	-0.88058	0.00186	-0.00258	0.00026	-0.24831	-0.00049
Q_{33}	633.2	-0.00102	-0.24578	0.17728	-0.07919	-0.00018	-0.02587
Q_{32}	722.0	0.00183	0.42177	-0.54770	0.50165	-0.00085	0.36695
Q_{31}	729.2	0.16002	-0.00047	0.00128	-0.00029	-0.92820	-0.00058
Q_{30}	758.4	0.00113	0.38109	-0.13103	0.20510	0.00049	-0.76047
Q_{29}	788.2	-0.02024	0.00098	0.00033	-0.00003	-0.04349	-0.00019
Q_{28}	812.4	0.00134	0.00031	-0.65745	-0.70640	-0.00060	0.00054
Q_{27}	853.3	0.00018	-0.07361	-0.12981	-0.06090	0.00049	-0.51314
Q_{26}	896.8	-0.00036	-0.77766	-0.41613	0.40237	-0.00042	-0.11544
Q_{25}	900.7	-0.01414	-0.00379	-0.00166	0.00226	0.03325	-0.00034
Q_{24}	934.2	-0.00007	-0.01630	0.09498	0.16826	-0.00111	-0.09529
Q_{23}	946.4	0.03025	-0.00104	0.00028	0.00099	-0.01962	-0.00045
Q_{22}	1087.9	-0.04270	0.00013	0.00019	-0.00027	0.06536	0.00010
Q_{21}	1110.3	-0.04155	-0.00038	-0.00005	0.00026	0.04893	0.00001
Q_{20}	1148.0	-0.02765	0.00000	-0.00009	-0.00012	0.10306	0.00027
Q_{19}	1159.6	0.03466	-0.00020	-0.00001	0.00009	-0.02568	-0.00008
Q_{18}	1238.7	-0.06617	-0.00001	-0.00021	-0.00003	0.10776	0.00027
Q_{17}	1269.9	0.02302	-0.00006	-0.00008	0.00029	-0.04693	0.00012
Q_{16}	1303.8	-0.01505	-0.00014	-0.00006	0.00002	0.04457	0.00000
Q_{15}	1353.2	0.03322	-0.00025	0.00005	0.00016	-0.07233	0.00016
Q_{14}	1390.2	-0.02164	-0.00001	-0.00029	0.00007	0.03444	0.00007
Q_{13}	1457.3	-0.04139	-0.00010	0.00004	-0.00011	0.06887	0.00019
Q_{12}	1487.0	-0.00951	0.00017	0.00018	-0.00029	-0.01276	0.00017
Q_{11}	1499.8	0.01827	-0.00003	0.00020	-0.00014	-0.00519	0.00010
Q_{10}	1546.3	0.05329	0.00011	0.00027	-0.00020	-0.07603	-0.00017
Q_9	1611.8	0.00967	0.00024	-0.00017	0.00011	-0.01001	-0.00006
Q_8	1657.9	0.00376	0.00018	-0.00026	0.00001	-0.00908	-0.00009
Q_7	2151.4	0.00345	0.00013	0.00002	-0.00012	-0.01111	0.00002
Q_6	3205.8	-0.00011	0.00003	0.00011	0.00011	0.00006	-0.00003
Q_5	3214.3	0.00032	-0.00017	-0.00010	0.00007	-0.00178	-0.00003
Q_4	3226.8	0.00162	-0.00008	-0.00012	-0.00010	-0.00318	-0.00001
Q_3	3267.6	-0.00072	0.00004	0.00006	-0.00008	0.00030	-0.00059
Q_2	3286.4	0.00027	0.00001	-0.00002	0.00004	-0.00046	0.00049
Q_1	3680.4	0.00011	0.00008	0.00003	0.00001	-0.00089	-0.00007

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Nr.	S_0/S_1	730.8	756.8	818.7	866.9	875.3	961.8
Q_{45}	105.2	-0.00188	0.00031	0.00243	0.00011	0.00012	0.00009
Q_{44}	139.2	0.00001	-0.00046	0.00001	-0.00490	-0.00187	0.00672
Q_{43}	225.7	-0.00319	0.00019	0.00675	-0.00039	0.00011	-0.00008
Q_{42}	263.9	0.00368	-0.00028	-0.00172	-0.00003	0.00003	0.00003
Q_{41}	379.1	-0.00012	0.00225	-0.00002	0.00934	0.00692	-0.04315
Q_{40}	400.2	0.00674	0.00110	0.00249	0.00036	-0.00038	0.00000
Q_{39}	417.1	-0.00009	0.00332	0.00014	-0.03055	-0.02328	0.03808
Q_{38}	421.3	0.01253	0.00003	-0.01756	-0.00027	-0.00005	0.00054
Q_{37}	481.7	-0.02175	-0.00011	0.00130	-0.00002	-0.00010	0.00003
Q_{36}	532.2	-0.00050	0.07922	-0.00015	0.02365	0.00845	-0.07501
Q_{35}	606.1	0.04667	0.00170	0.09385	0.00103	0.00015	-0.00065
Q_{34}	613.8	-0.00060	0.07116	-0.00053	0.04060	0.06488	-0.10332
Q_{33}	633.2	-0.06906	0.00031	0.00777	0.00034	-0.00019	-0.00004
Q_{32}	722.0	-0.00796	0.00014	0.22737	-0.00003	0.00017	0.00047
Q_{31}	729.2	-0.00115	-0.00877	0.00031	-0.11821	-0.09212	0.23107
Q_{30}	758.4	-0.08897	0.00029	-0.43144	-0.00039	-0.00033	0.00051
Q_{29}	788.2	0.00421	-0.96601	-0.00055	0.22391	-0.03395	-0.04762
Q_{28}	812.4	0.18636	0.00078	-0.13645	0.00002	0.00007	0.00022
Q_{27}	853.3	-0.04174	-0.00088	0.83882	-0.00033	0.00065	-0.00016
Q_{26}	896.8	-0.04242	0.00005	-0.17467	0.00442	-0.00221	0.00056
Q_{25}	900.7	0.00265	-0.20919	-0.00127	-0.91938	0.24734	-0.19174
Q_{24}	934.2	0.97266	0.00466	0.01325	0.00119	-0.00328	-0.00056
Q_{23}	946.4	0.00285	-0.00067	-0.00069	0.17234	0.89459	0.36155
Q_{22}	1087.9	0.00003	-0.01671	-0.00006	-0.06978	-0.16791	0.41568
Q_{21}	1110.3	0.00030	-0.00934	0.00014	-0.08927	-0.13967	0.26997
Q_{20}	1148.0	0.00051	-0.07131	0.00031	-0.07363	0.03033	0.37078
Q_{19}	1159.6	0.00016	-0.00569	-0.00008	0.01601	0.09083	-0.19212
Q_{18}	1238.7	0.00013	-0.04775	0.00044	-0.15163	-0.16489	0.41320
Q_{17}	1269.9	-0.00003	0.02908	0.00011	0.04789	0.05181	-0.15400
Q_{16}	1303.8	0.00017	-0.01054	0.00005	-0.00407	-0.02476	0.09337
Q_{15}	1353.2	-0.00012	0.01453	0.00018	0.05846	0.05280	-0.20979
Q_{14}	1390.2	0.00043	0.02342	0.00018	-0.05615	-0.03456	0.10159
Q_{13}	1457.3	0.00001	-0.03932	0.00014	-0.04637	-0.07581	0.20059
Q_{12}	1487.0	-0.00045	0.01587	0.00013	0.03483	-0.04564	-0.00270
Q_{11}	1499.8	0.00005	-0.01205	-0.00022	0.00884	0.09930	-0.02438
Q_{10}	1546.3	-0.00021	0.01118	0.00024	0.05579	0.11504	-0.19379
Q_9	1611.8	-0.00010	0.00406	-0.00018	0.01260	0.02278	-0.02509
Q_8	1657.9	-0.00012	0.00329	-0.00005	0.02255	0.03192	-0.01397
Q_7	2151.4	0.00015	-0.00308	0.00001	0.00584	0.01379	-0.01954
Q_6	3205.8	0.00012	0.00138	0.00000	-0.00013	-0.00203	-0.00024
Q_5	3214.3	-0.00003	0.00026	0.00001	-0.00012	-0.00031	-0.00109
Q_4	3226.8	0.00007	0.00039	-0.00000	0.00085	-0.00011	-0.00276
Q_3	3267.6	-0.00008	-0.00051	0.00011	-0.00092	-0.00011	0.00303
Q_2	3286.4	0.00008	0.00030	-0.00027	0.00001	0.00103	-0.00186
Q_1	3680.4	-0.00003	0.00093	-0.00006	0.00210	0.00029	-0.00180

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Nr.	S_0/S_1	1062.8	1087.1	1107.3	1170.5	1239.0	1272.6
Q_{45}	105.2	-0.00023	0.00025	0.00008	0.00019	0.00016	0.00024
Q_{44}	139.2	0.00365	-0.00050	-0.00070	0.00436	0.00167	0.00013
Q_{43}	225.7	0.00002	-0.00016	-0.00000	-0.00013	-0.00006	0.00013
Q_{42}	263.9	0.00019	-0.00003	0.00021	0.00034	0.00003	-0.00010
Q_{41}	379.1	0.00600	0.00147	-0.01327	-0.01041	-0.00303	-0.00562
Q_{40}	400.2	-0.00032	-0.00018	-0.00018	0.00004	-0.00007	0.00018
Q_{39}	417.1	0.00881	0.01189	0.00898	0.01756	0.01243	0.01319
Q_{38}	421.3	0.00015	-0.00015	0.00005	0.00016	0.00008	-0.00021
Q_{37}	481.7	0.00022	-0.00006	-0.00010	-0.00002	-0.00006	-0.00013
Q_{36}	532.2	-0.03509	0.00385	0.01572	-0.02071	-0.00556	0.00983
Q_{35}	606.1	0.00000	-0.00013	-0.00007	-0.00017	-0.00037	0.00025
Q_{34}	613.8	-0.01679	-0.00501	-0.01581	-0.02814	-0.00671	0.00219
Q_{33}	633.2	0.00022	-0.00022	-0.00007	-0.00013	-0.00002	0.00003
Q_{32}	722.0	-0.00001	0.00008	-0.00006	0.00000	-0.00042	-0.00009
Q_{31}	729.2	0.04749	-0.03981	-0.02097	0.01597	-0.00416	-0.02072
Q_{30}	758.4	0.00023	-0.00009	-0.00010	-0.00012	0.00021	0.00017
Q_{29}	788.2	-0.02173	0.02997	0.02652	0.01193	0.01001	-0.00134
Q_{28}	812.4	0.00011	0.00020	0.00006	0.00001	0.00008	0.00004
Q_{27}	853.3	-0.00025	0.00013	0.00005	0.00005	-0.00014	-0.00012
Q_{26}	896.8	-0.00014	-0.00057	-0.00020	-0.00008	-0.00018	0.00024
Q_{25}	900.7	-0.06764	0.01992	0.03363	-0.01525	-0.00512	-0.02374
Q_{24}	934.2	-0.00001	-0.00060	-0.00017	-0.00011	-0.00011	0.00018
Q_{23}	946.4	-0.02730	0.10573	0.06274	0.11101	0.00881	0.01263
Q_{22}	1087.9	-0.75958	0.29464	-0.29531	-0.11415	-0.06585	-0.05048
Q_{21}	1110.3	0.42355	0.73694	0.27126	-0.27686	-0.02630	-0.00538
Q_{20}	1148.0	0.23433	-0.45878	-0.25699	-0.68371	0.06375	0.11594
Q_{19}	1159.6	0.27037	0.28646	-0.84615	0.11246	-0.08518	0.15253
Q_{18}	1238.7	0.16177	-0.12919	-0.05494	0.57263	0.34631	0.27575
Q_{17}	1269.9	-0.08571	0.12515	-0.04797	-0.17412	0.91278	-0.15260
Q_{16}	1303.8	0.11883	-0.06150	-0.14821	0.11460	-0.03046	-0.86170
Q_{15}	1353.2	-0.08261	0.13814	-0.01968	-0.09300	0.09134	0.22733
Q_{14}	1390.2	-0.06802	-0.03467	0.04433	0.01586	0.03435	0.03822
Q_{13}	1457.3	0.07430	-0.04178	-0.03188	0.10489	0.01977	0.00992
Q_{12}	1487.0	-0.11771	-0.03050	0.12360	-0.03791	-0.06740	0.22258
Q_{11}	1499.8	0.02456	-0.05418	0.01745	-0.04026	-0.11963	-0.09744
Q_{10}	1546.3	-0.15078	0.01754	0.00056	-0.14558	0.00572	0.05720
Q_9	1611.8	-0.01993	-0.02890	0.02678	-0.00277	-0.00667	0.03857
Q_8	1657.9	-0.06067	0.01113	0.05698	0.00829	0.01584	0.01844
Q_7	2151.4	-0.00559	-0.00090	-0.00067	0.00124	-0.00498	0.00222
Q_6	3205.8	-0.00136	-0.00081	0.00248	-0.00059	0.00232	-0.00382
Q_5	3214.3	0.00100	0.00206	-0.00120	0.00306	0.00073	-0.00045
Q_4	3226.8	-0.00496	-0.00200	0.00421	-0.00267	-0.00365	0.00281
Q_3	3267.6	-0.00001	0.00184	0.00107	-0.00066	-0.00258	-0.00040
Q_2	3286.4	-0.00104	-0.00099	-0.00154	0.00112	-0.00189	-0.00090
Q_1	3680.4	-0.00107	-0.00016	0.00078	0.00061	-0.00179	0.00050

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Nr.	S_0/S_1	1304.8	1354.0	1385.2	1430.5	1444.0	1526.0
Q_{45}	105.2	-0.00011	0.00004	0.00013	0.00010	0.00002	-0.00008
Q_{44}	139.2	0.00018	0.00231	0.00285	0.00083	0.00015	0.00030
Q_{43}	225.7	-0.00008	0.00010	0.00010	0.00003	-0.00016	-0.00007
Q_{42}	263.9	0.00005	-0.00005	0.00009	0.00010	0.00015	-0.00002
Q_{41}	379.1	-0.00712	-0.00263	0.00408	0.00312	-0.00273	0.00240
Q_{40}	400.2	0.00010	0.00030	-0.00003	0.00042	-0.00036	-0.00036
Q_{39}	417.1	-0.00406	0.00747	0.01738	0.00374	0.01419	-0.00255
Q_{38}	421.3	0.00002	-0.00001	0.00007	0.00006	0.00030	0.00000
Q_{37}	481.7	0.00006	0.00004	-0.00007	-0.00005	0.00002	0.00001
Q_{36}	532.2	0.00360	-0.03050	-0.00920	0.00218	0.00989	-0.00468
Q_{35}	606.1	0.00014	-0.00018	0.00037	0.00019	-0.00008	0.00027
Q_{34}	613.8	-0.00384	-0.02730	0.00321	0.00522	-0.01060	-0.00129
Q_{33}	633.2	0.00022	-0.00001	-0.00000	-0.00000	0.00003	0.00012
Q_{32}	722.0	0.00025	-0.00015	0.00013	-0.00012	-0.00004	-0.00009
Q_{31}	729.2	0.01343	0.02703	0.00287	-0.01413	0.00707	0.00180
Q_{30}	758.4	-0.00021	-0.00008	-0.00008	-0.00031	-0.00000	-0.00017
Q_{29}	788.2	0.00184	0.01326	-0.02271	0.00441	0.01527	-0.00036
Q_{28}	812.4	0.00000	-0.00002	0.00014	-0.00001	-0.00002	-0.00001
Q_{27}	853.3	0.00021	0.00003	0.00013	-0.00016	0.00019	0.00025
Q_{26}	896.8	0.00015	-0.00025	-0.00005	0.00001	-0.00038	-0.00005
Q_{25}	900.7	0.00849	-0.00040	-0.02093	0.00915	0.01999	0.01097
Q_{24}	934.2	0.00015	-0.00042	0.00007	-0.00010	-0.00034	0.00010
Q_{23}	946.4	-0.00019	0.04540	-0.02094	0.03089	0.05405	-0.00555
Q_{22}	1087.9	0.00338	-0.07131	0.08651	0.00308	0.00983	0.03931
Q_{21}	1110.3	-0.03067	-0.08121	-0.05557	0.02553	-0.07290	0.01107
Q_{20}	1148.0	-0.09902	-0.06971	-0.01913	0.04360	0.02634	-0.00259
Q_{19}	1159.6	0.10652	0.03081	-0.14531	-0.02677	-0.00863	0.02887
Q_{18}	1238.7	-0.19717	-0.34393	-0.03553	0.07184	-0.08873	-0.00978
Q_{17}	1269.9	0.20249	0.02477	-0.02858	-0.08719	0.01016	0.06142
Q_{16}	1303.8	-0.29221	-0.10954	-0.26357	0.01935	0.00273	0.02439
Q_{15}	1353.2	-0.80495	-0.03122	0.08359	-0.30333	0.16715	0.02970
Q_{14}	1390.2	-0.19630	0.49705	-0.48005	-0.27250	-0.01941	-0.11161
Q_{13}	1457.3	0.10962	0.47750	0.11224	-0.38808	-0.48200	-0.09114
Q_{12}	1487.0	0.21476	-0.22327	-0.74945	-0.12823	0.13604	0.15840
Q_{11}	1499.8	0.15014	-0.47700	0.14085	-0.72938	-0.20019	0.19549
Q_{10}	1546.3	-0.16690	-0.25566	-0.18770	0.26030	-0.74742	-0.32925
Q_9	1611.8	-0.13108	0.15715	-0.02568	0.22053	-0.31942	0.88903
Q_8	1657.9	0.00286	-0.05386	-0.16452	-0.02062	-0.03942	-0.09516
Q_7	2151.4	-0.00516	-0.02241	0.00310	0.01061	-0.01732	0.00006
Q_6	3205.8	0.00059	-0.00140	0.00416	-0.00076	0.00425	-0.00505
Q_5	3214.3	-0.00437	0.00222	0.00258	0.00253	-0.00219	0.00125
Q_4	3226.8	-0.00419	-0.00159	-0.00450	0.00144	0.00501	-0.00212
Q_3	3267.6	0.00150	0.00175	0.00072	0.00430	-0.00103	0.00033
Q_2	3286.4	0.00334	-0.00177	0.00353	-0.00414	0.00422	0.00379
Q_1	3680.4	0.00105	0.00211	-0.00099	-0.00123	-0.00063	-0.00229

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Nr.	S_0/S_1	1617.7	1630.2	2085.1	3218.6	3233.1	3234.4
Q_{45}	105.2	0.00004	-0.00005	-0.00036	-0.00001	0.00001	-0.00000
Q_{44}	139.2	0.00244	-0.00005	-0.00215	-0.00009	-0.00000	0.00034
Q_{43}	225.7	-0.00013	0.00004	0.00012	0.00000	0.00002	0.00003
Q_{42}	263.9	-0.00016	-0.00017	-0.00055	-0.00001	0.00002	0.00002
Q_{41}	379.1	0.00296	0.00149	-0.00072	0.00045	-0.00030	-0.00017
Q_{40}	400.2	0.00004	0.00023	0.00006	0.00003	-0.00007	0.00002
Q_{39}	417.1	-0.01196	0.00348	0.00581	-0.00009	-0.00078	-0.00058
Q_{38}	421.3	-0.00057	-0.00011	0.00025	0.00000	-0.00004	0.00000
Q_{37}	481.7	0.00022	0.00012	0.00090	-0.00001	0.00003	-0.00001
Q_{36}	532.2	-0.04971	-0.01070	-0.00660	0.00117	0.00074	-0.00067
Q_{35}	606.1	0.00008	0.00011	0.00020	0.00001	0.00000	0.00003
Q_{34}	613.8	-0.01042	-0.00165	-0.00150	0.00082	0.00105	0.00027
Q_{33}	633.2	0.00045	0.00031	-0.00042	0.00001	-0.00005	-0.00001
Q_{32}	722.0	0.00005	-0.00019	-0.00000	0.00000	0.00001	0.00001
Q_{31}	729.2	0.00290	0.00594	0.00586	-0.00070	-0.00068	-0.00270
Q_{30}	758.4	-0.00003	-0.00025	-0.00002	-0.00002	0.00001	0.00003
Q_{29}	788.2	0.02807	0.00215	0.00369	0.00141	-0.00031	-0.00023
Q_{28}	812.4	-0.00003	-0.00016	0.00010	0.00008	-0.00014	-0.00014
Q_{27}	853.3	-0.00004	-0.00001	-0.00001	0.00001	0.00001	-0.00006
Q_{26}	896.8	0.00018	-0.00002	-0.00009	0.00003	0.00010	-0.00019
Q_{25}	900.7	-0.04896	-0.01009	0.00161	0.00016	-0.00043	0.00006
Q_{24}	934.2	-0.00034	0.00009	0.00010	-0.00017	-0.00001	-0.00001
Q_{23}	946.4	-0.02899	-0.04542	0.00664	0.00154	-0.00044	0.00039
Q_{22}	1087.9	0.00512	0.00043	-0.00649	-0.00076	-0.00047	0.00016
Q_{21}	1110.3	0.02951	0.01082	-0.00982	0.00175	0.00211	0.00135
Q_{20}	1148.0	-0.02879	0.03341	-0.01007	0.00045	-0.00210	0.00211
Q_{19}	1159.6	0.02458	0.04190	0.00240	0.00585	0.00284	0.00149
Q_{18}	1238.7	0.06876	0.01016	-0.00481	0.00250	0.00377	0.00112
Q_{17}	1269.9	0.00147	-0.02065	-0.00172	-0.00160	0.00273	0.00302
Q_{16}	1303.8	-0.14249	-0.05545	-0.00037	-0.00171	0.00147	0.00063
Q_{15}	1353.2	-0.24695	-0.07652	0.00818	-0.00266	-0.00282	-0.00510
Q_{14}	1390.2	0.59427	0.10617	-0.01987	0.00480	0.00137	-0.00218
Q_{13}	1457.3	-0.50864	-0.13396	-0.01097	0.00029	0.00148	0.00431
Q_{12}	1487.0	-0.35438	-0.25415	0.00734	-0.00189	-0.00954	-0.00046
Q_{11}	1499.8	0.27019	0.07704	0.00687	0.00186	0.00123	0.00338
Q_{10}	1546.3	0.10033	-0.09534	0.03408	0.00194	-0.00025	-0.00244
Q_9	1611.8	0.04404	0.09617	0.00308	0.00786	0.00212	-0.00132
Q_8	1657.9	-0.28690	0.93054	-0.03065	0.00243	-0.00268	0.00038
Q_7	2151.4	0.00322	-0.03466	-0.99837	0.00157	-0.00196	-0.00069
Q_6	3205.8	-0.00326	-0.00404	0.00219	0.95568	-0.27809	-0.09549
Q_5	3214.3	0.00556	0.00057	0.00071	-0.13093	-0.69356	0.70825
Q_4	3226.8	-0.00390	-0.00182	-0.00116	0.26318	0.66437	0.69936
Q_3	3267.6	0.00462	0.00294	0.00046	-0.00675	0.00280	0.00629
Q_2	3286.4	0.00045	0.00089	-0.00124	0.00750	0.00877	-0.00423
Q_1	3680.4	-0.00369	-0.00083	-0.00011	0.00033	0.00034	0.00014

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Nr.	S_0/S_1	3265.6	3285.1	3672.3
Q_{45}	105.2	-0.00003	-0.00004	-0.00004
Q_{44}	139.2	0.00029	0.00017	0.00014
Q_{43}	225.7	-0.00005	-0.00007	-0.00014
Q_{42}	263.9	0.00003	0.00005	-0.00002
Q_{41}	379.1	0.00047	-0.00009	0.00059
Q_{40}	400.2	0.00007	-0.00001	-0.00082
Q_{39}	417.1	0.00027	0.00047	0.00001
Q_{38}	421.3	0.00001	0.00002	-0.00012
Q_{37}	481.7	-0.00000	0.00003	0.00008
Q_{36}	532.2	0.00015	-0.00038	0.00008
Q_{35}	606.1	0.00014	0.00013	-0.00023
Q_{34}	613.8	-0.00041	-0.00032	-0.00017
Q_{33}	633.2	0.00002	0.00004	-0.00006
Q_{32}	722.0	0.00020	0.00026	0.00002
Q_{31}	729.2	-0.00027	0.00023	-0.00031
Q_{30}	758.4	-0.00028	-0.00034	-0.00011
Q_{29}	788.2	-0.00027	-0.00048	0.00041
Q_{28}	812.4	0.00002	0.00005	-0.00001
Q_{27}	853.3	-0.00023	-0.00059	0.00004
Q_{26}	896.8	0.00004	0.00002	0.00002
Q_{25}	900.7	-0.00042	0.00039	0.00151
Q_{24}	934.2	0.00001	0.00004	0.00003
Q_{23}	946.4	-0.00080	-0.00020	-0.00031
Q_{22}	1087.9	-0.00201	-0.00008	0.00087
Q_{21}	1110.3	-0.00192	-0.00388	0.00158
Q_{20}	1148.0	0.00020	-0.00155	0.00209
Q_{19}	1159.6	0.00021	0.00162	0.00007
Q_{18}	1238.7	0.00090	-0.00198	0.00286
Q_{17}	1269.9	0.00257	0.00068	0.00102
Q_{16}	1303.8	0.00135	-0.00052	0.00057
Q_{15}	1353.2	0.00478	0.00117	-0.00079
Q_{14}	1390.2	-0.00144	-0.00313	0.00065
Q_{13}	1457.3	0.00271	-0.00086	-0.00330
Q_{12}	1487.0	0.00352	0.00070	-0.00228
Q_{11}	1499.8	-0.00010	0.00566	0.00124
Q_{10}	1546.3	0.00145	-0.00560	-0.00083
Q_9	1611.8	-0.00201	-0.00010	0.00196
Q_8	1657.9	-0.00092	-0.00050	-0.00081
Q_7	2151.4	0.00021	0.00135	-0.00016
Q_6	3205.8	0.00581	0.00739	-0.00022
Q_5	3214.3	-0.00004	-0.01065	0.00019
Q_4	3226.8	-0.00575	0.00317	-0.00044
Q_3	3267.6	0.94773	0.31879	-0.00018
Q_2	3286.4	0.31885	-0.94767	-0.00195
Q_1	3680.4	0.00081	-0.00178	0.99998

Table S3: Experimental intensities of the assigned bands in the DF and LIF spectra relative to the strongest band in each spectrum. Keep in mind, that the mode numbering is different in the S_0 and the S_1 state as can be inferred from Table 1 of the main text. No 0,0 intensities for the fluorescence emission spectra is given since they might be contaminated by laser stray light and have not been used in the FC fit.

	Emission					Abs.
Mode	Origin	+350	+666	+753	+884	
$0,0$						0.80
Q_{45}^2	0.05	0.001		0.01		
Q_{44}	0.15	0.004	0.06	0.02		
Q_{43}^2	0.03					
Q_{41}	0.02	1.000				
Q_{41}^2			0.07			
$Q_{41}+Q_{36}$		0.14				
$Q_{41}+Q_{34}$					0.49	
$Q_{41}+Q_{31}$		0.15				
$Q_{41}+Q_{29}$		0.24				
$Q_{41}+Q_{23}$		0.06				
$Q_{41}+Q_{22}$		0.10				
$Q_{41}+Q_{18}$		0.08				
$Q_{41}+Q_{17}$		0.15				
Q_{40}^2	0.12	0.010		0.10		
Q_{39}	0.05	0.001		0.05	0.04	0.68
$Q_{39}+Q_{31}$		0.03				
$Q_{39}+Q_{18}$		0.04				
Q_{38}^2			0.20			
Q_{37}^2	0.08			0.02		0.32
Q_{36}	0.63			0.15	0.12	0.36
Q_{32}^2	0.40			0.10		
Q_{31}	0.59	0.050	1.0	0.08	0.06	
Q_{30}^2		0.020		0.15	0.17	
Q_{29}	1.00	0.030		1.00	0.18	0.64
Q_{28}^2	0.08	0.040				
Q_{26}						1.00
Q_{25}	0.10					
Q_{23}					1.00	0.89
Q_{22}	0.42	0.010	0.05	0.09	0.02	0.50
Q_{20}					0.11	
Q_{18}	0.38			0.03	0.14	
Q_{17}	0.62	0.030	0.07			
Q_{16}	0.23			0.12	0.79	
Q_{15}	0.06				0.06	
Q_{13}	0.27					
Q_{11}		0.020		0.15	0.17	
Q_{10}	0.21					
Q_8	0.05	0.150				
Q_7	0.06			0.06		