Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Online material for: Structures, Dipole Moments and Excited State Lifetime of Isolated 4-Cyanoindole in its Ground and Lowest Electronically Excited Singlet States.

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The supporting online material contains:

- A table, containing the Cartesian coordinates in Bohr of 4-cyanoindole in the S_0 state from SCS-CC2/cc-pVTZ calculations.
- A table, containing the Cartesian coordinates in Bohr of 4-cyanoindole in the S_1 state from SCS-CC2/cc-pVTZ calculations.
- A figure, containing the Duschinsky matrix of the 45 vibrational modes of 3-cyanoindole.
- A figure, containing the Duschinsky matrix of the 45 vibrational modes of 5-cyanoindole.
- A figure, containing an expanded view of the rotationally resolved electronic spectrum of the electronic origin of 4-cyanoindole.
- A figure, containing the rotationally resolved electronic spectrum of the electronic origin of 1-deuterated 4-cyanoindole.
- A figure, containing the rotationally resolved electronic spectrum of the electronic origin of 2-deuterated 4-cyanoindole.
- A figure, containing the rotationally resolved electronic spectrum of the electronic origin of 3-deuterated 4-cyanoindole.
- A figure, containing the frontier orbitals involved in the S_1 and S_2 excitation.
- A figure, containing the electron density difference plots of 3-cyanoindole, 4-cyanoindole, and 5-cyanoindole.

Table S1 SCS CC2/cc-pVTZ calculated optimized S_0 cartesian coordinates of 4-Cyanoindole (in bohr).

C	-0.82504608	-3.87198701	0.00034434
C	1.83519861	-3.85210200	0.00033732
C	3.18786743	-1.59899921	0.00019318
C	1.80605976	0.65619474	-0.00012977
N	2.61329577	3.12879219	-0.00018408
C	0.53763349	4.71262771	-0.00044918
C	-1.64175633	3.29813955	-0.00038107
C	-0.87663304	0.70490427	-0.00016181
C	-2.19025154	-1.61759864	0.00015035
H	-1.83187524	-5.65068808	0.00041866
H	2.84224224	-5.63079393	0.00035979
H	5.23386112	-1.59957638	0.00043898
H	0.78397478	6.73375545	-0.00067922
H	-3.54507475	4.01860007	-0.00044386
H	4.42491253	3.69671743	-0.00007359
C	-4.90169006	-1.63392783	0.00027832
N	-7.12489769	-1.60998934	0.00037865

Table S2 SCS CC2/cc-pVTZ calculated optimized S_1 cartesian coordinates of 4-Cyanoindole (in bohr).

C	-0.82507474	-3.93152508	0.00032150
C	1.82630119	-3.85560603	0.00037094
C	3.27188112	-1.57150725	0.00024608
C	1.78860280	0.63627276	0.00009284
N	2.59454221	3.19379366	-0.00012519
C	0.60392348	4.74034608	-0.00034306
C	-1.63647151	3.20765677	-0.00025661
C	-0.88430930	0.67027110	0.00001317
C	-2.30936200	-1.66335424	0.00012664
H	-1.76825238	-5.74427165	0.00044258
H	2.83823761	-5.63468372	0.00052278
H	5.31217374	-1.56518571	0.00023251
H	0.80199664	6.76728508	-0.00054173
H	-3.54348946	3.93109255	-0.00039221
H	4.41657538	3.75438147	-0.00017546
C	-4.95943730	-1.60199025	-0.00000610
N	-7.20001646	-1.44890655	-0.00013166

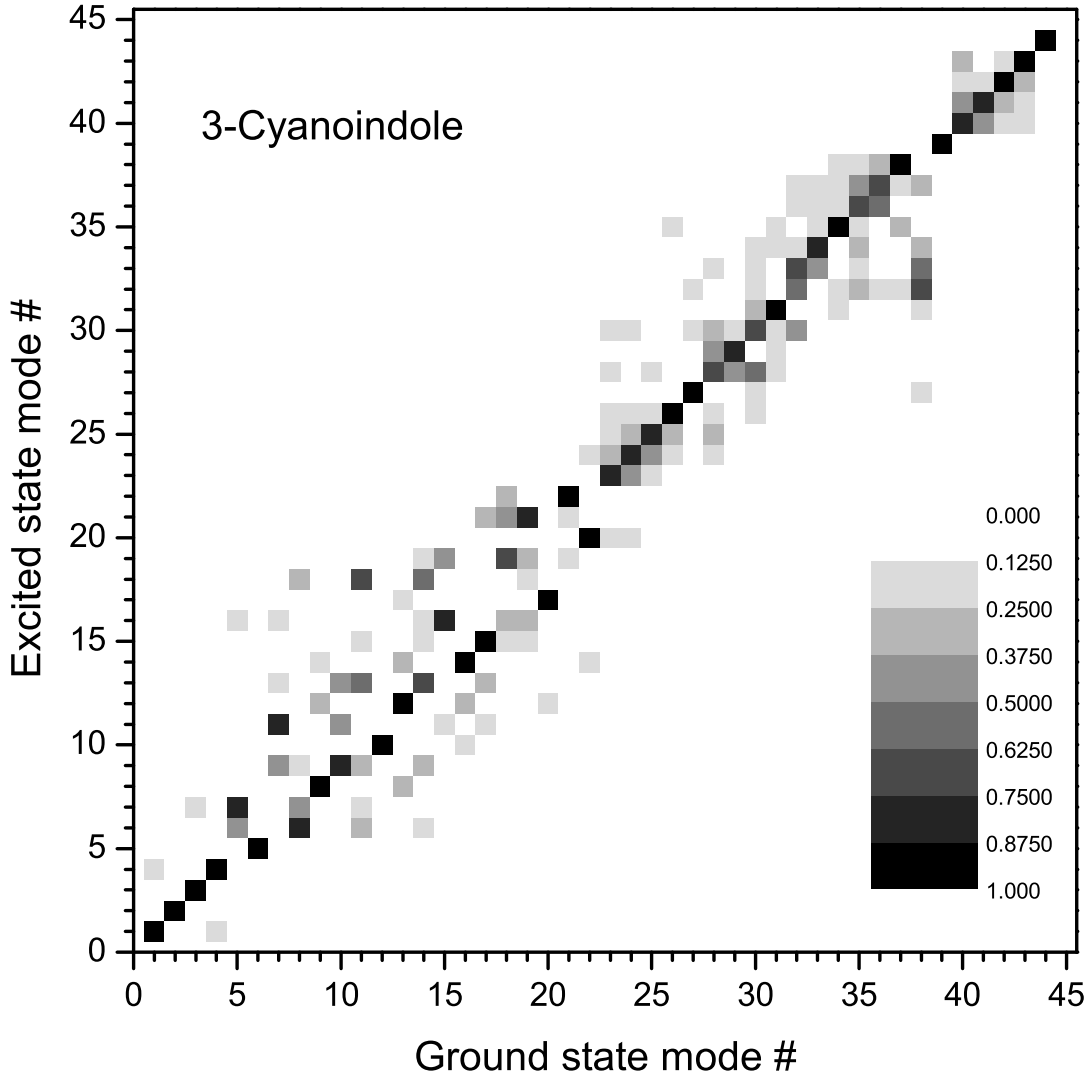

Figure S1 Duschinsky matrix of the 45 vibrational modes of 3-cyanoindole.

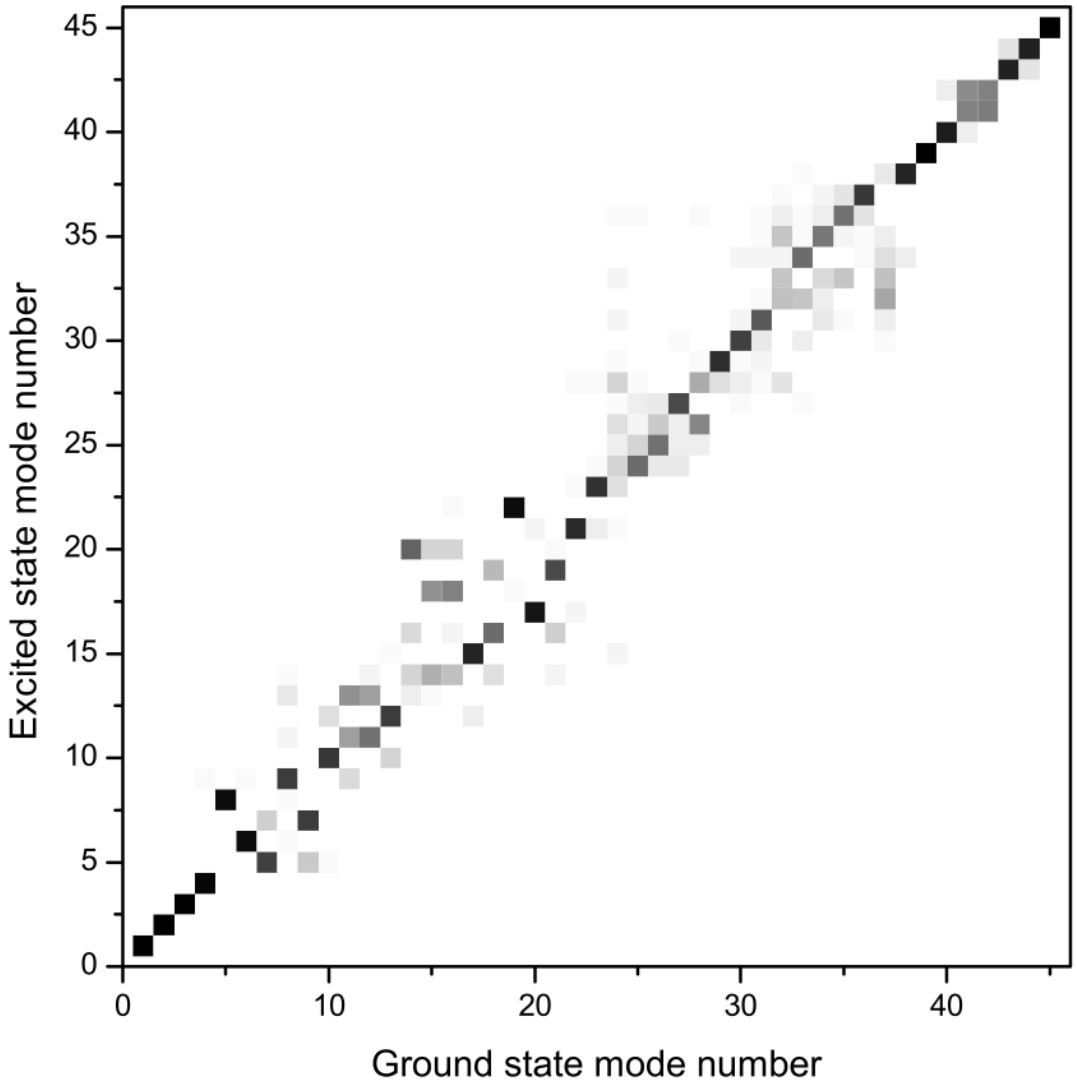

Figure S2 Duschinsky matrix of the 45 vibrational modes of 5-cyanoindole.

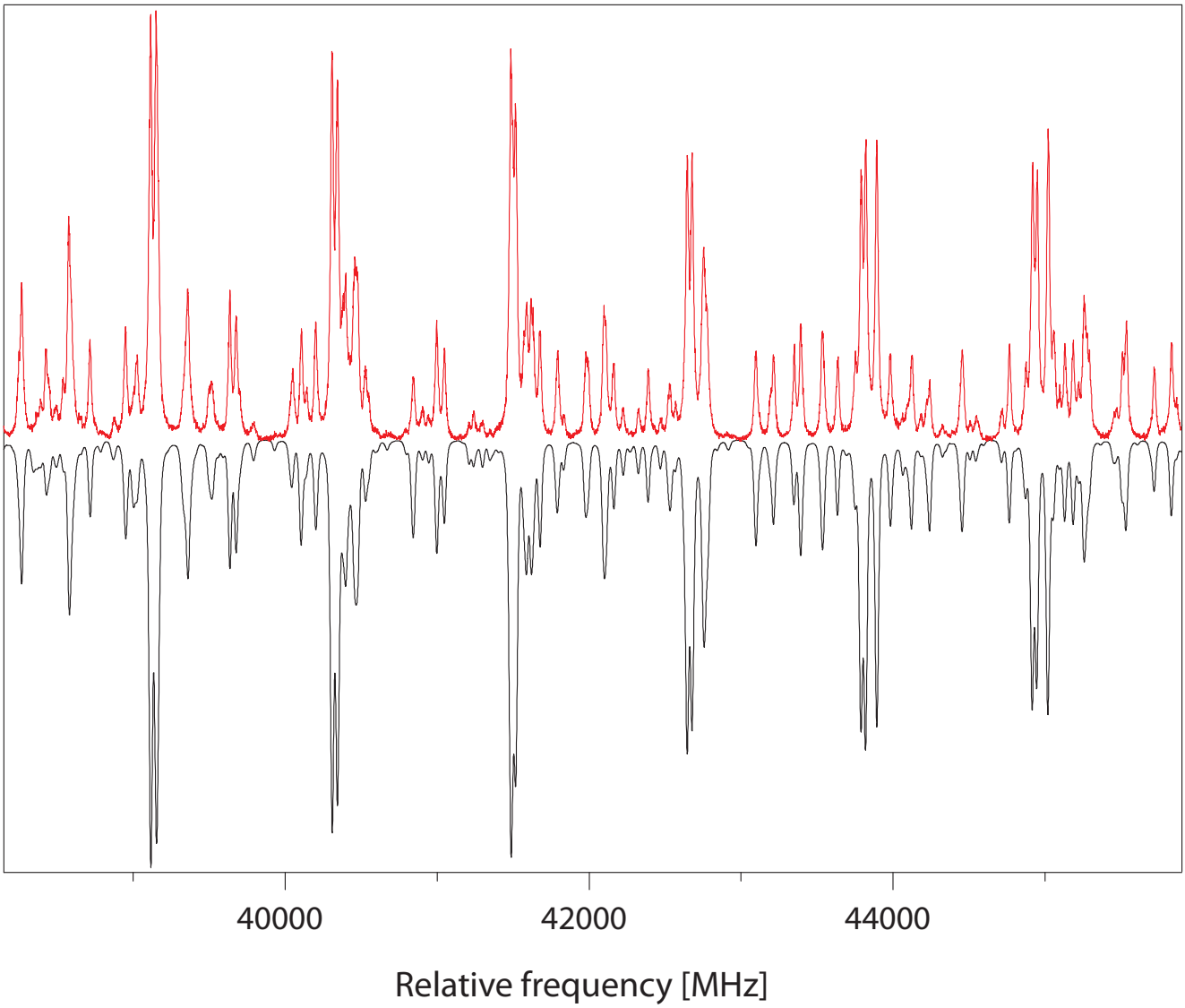

Figure S3 Expanded view of the rotationally resolved electronic spectrum of the electronic origin of 4-cyanoindole along with a fit of the line form parameters to determine the fluorescence lifetime.

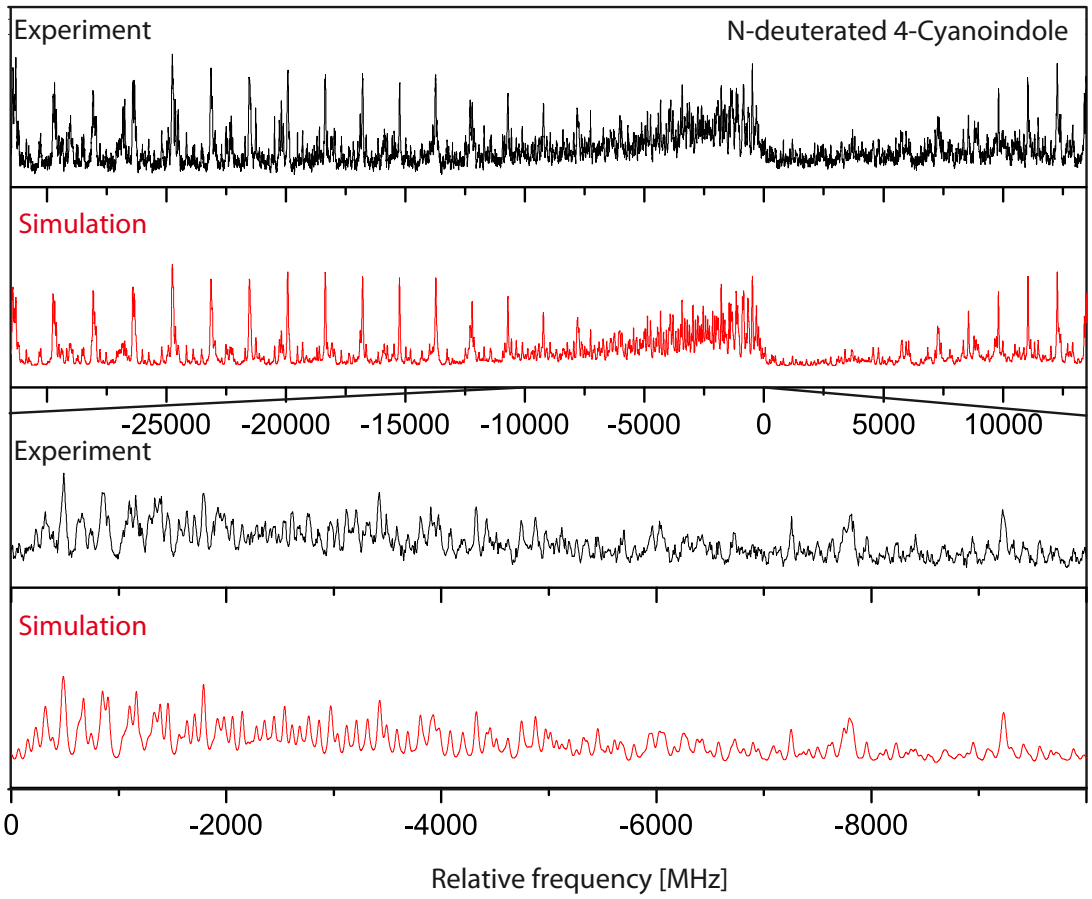

Figure S4 Rotationally resolved electronic spectrum of the electronic origin of N-deuterated 4-cyanoindole

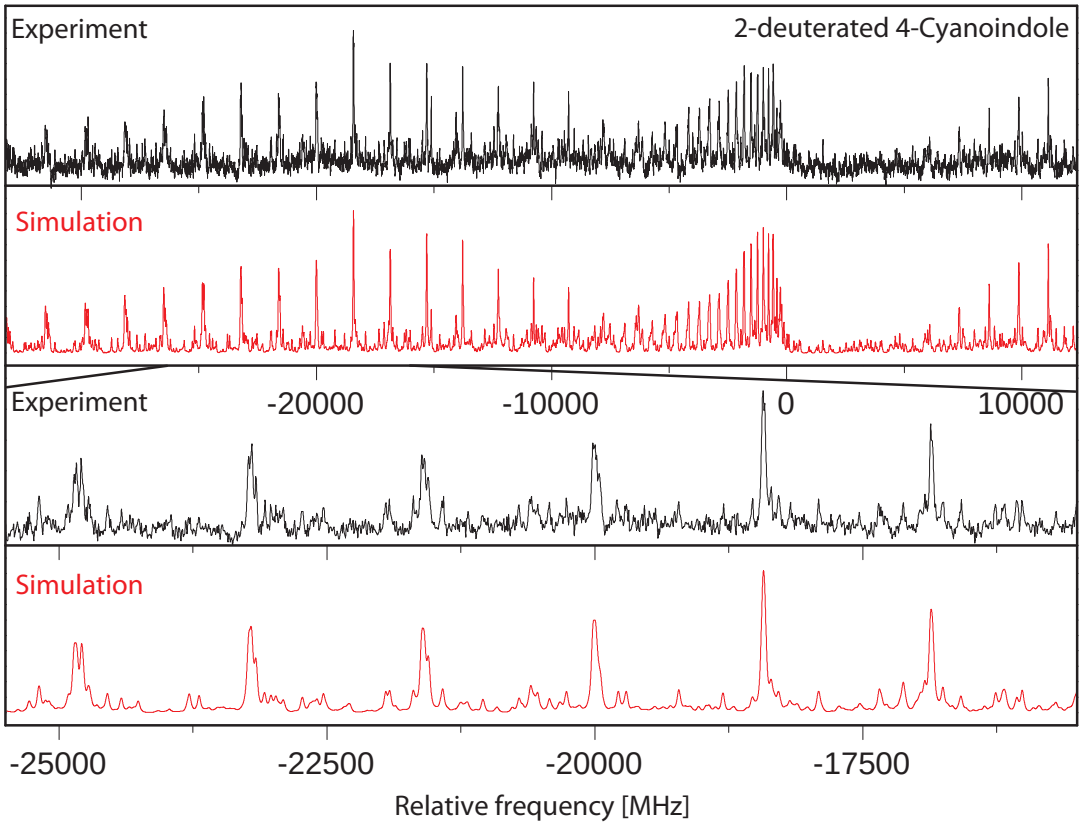

Figure S5 Rotationally resolved electronic spectrum of the electronic origin of 2-deuterated 4-cyanoindole

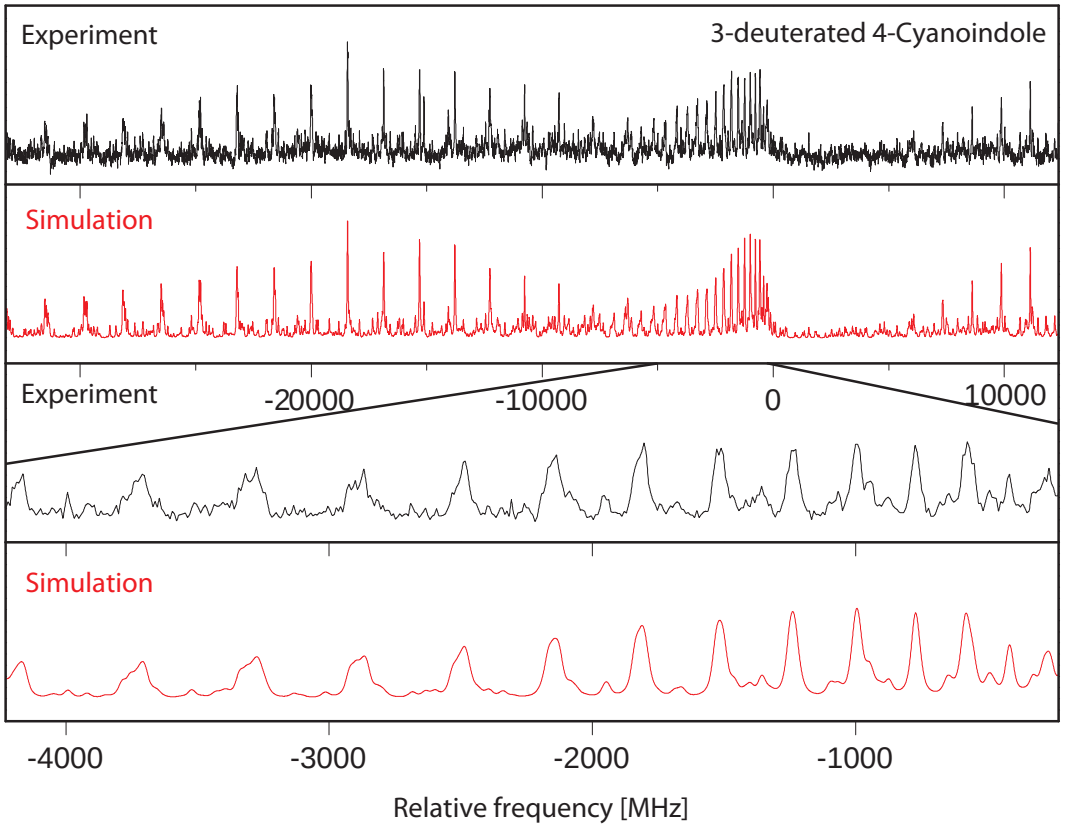

Figure S6 Rotationally resolved electronic spectrum of the electronic origin of 3-deuterated 4-cyanoindole

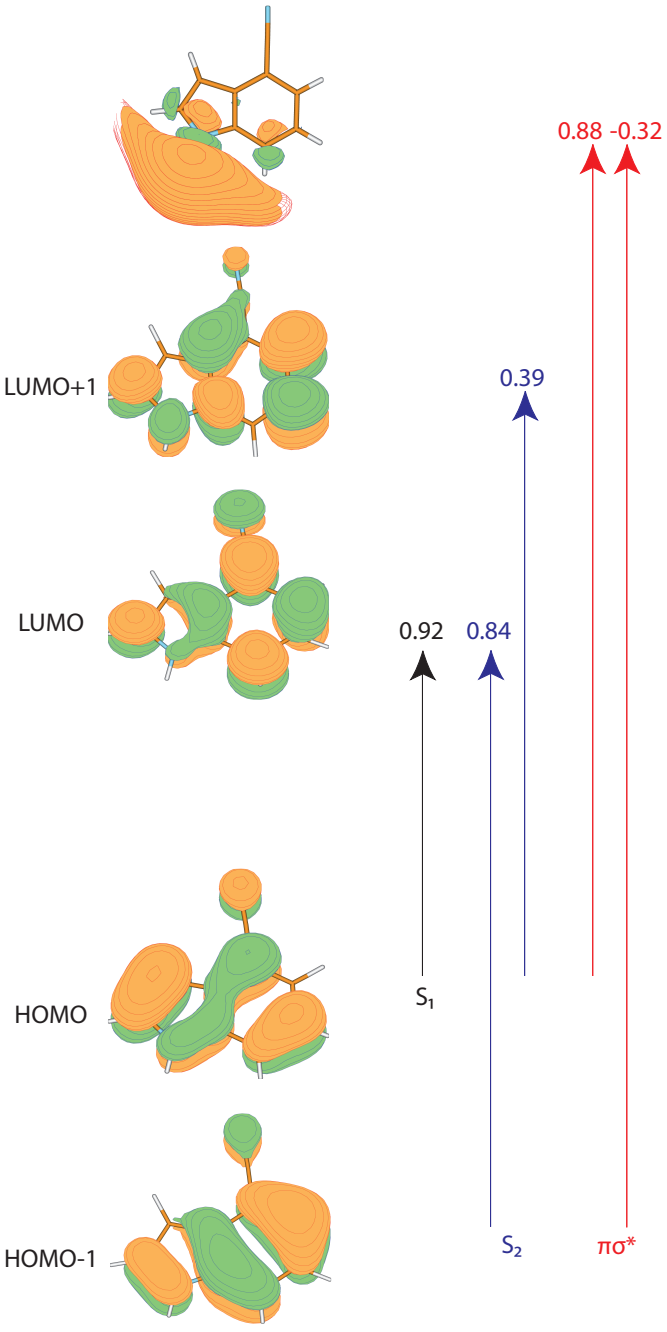

Figure S7 Frontier orbitals involved in the S_1 and S_2 excitation and leading contributions to the excitations.

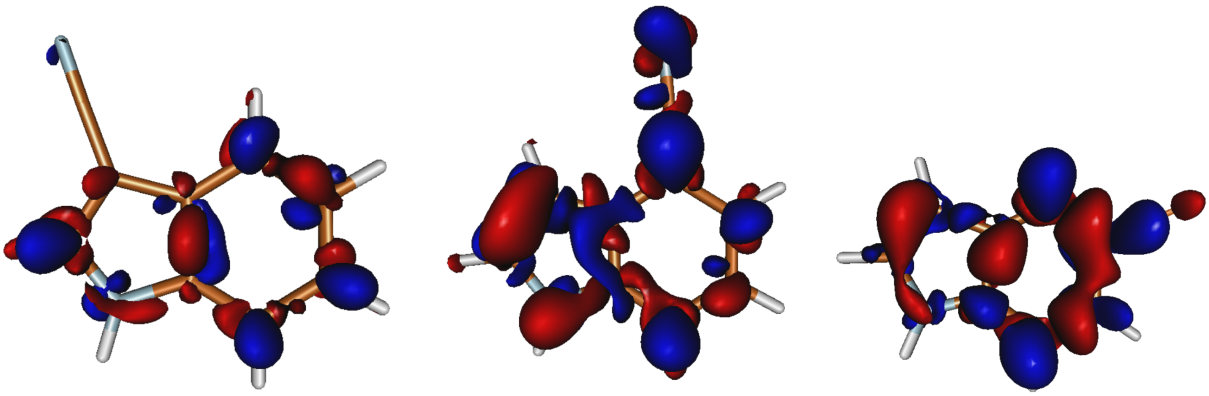

Figure S8 Electron density difference plots of 3-cyanoindole, 4-cyanoindole, and 5-cyanoindole.