Electronic Supplementary Material for PCCP

—*Phys. Chem. Chem. Phys.* —

Sub-picosecond fluorescence evolution of amino-cyano-stilbenes in methanol: polar solvation obeys continuum theory without evidence of twisting

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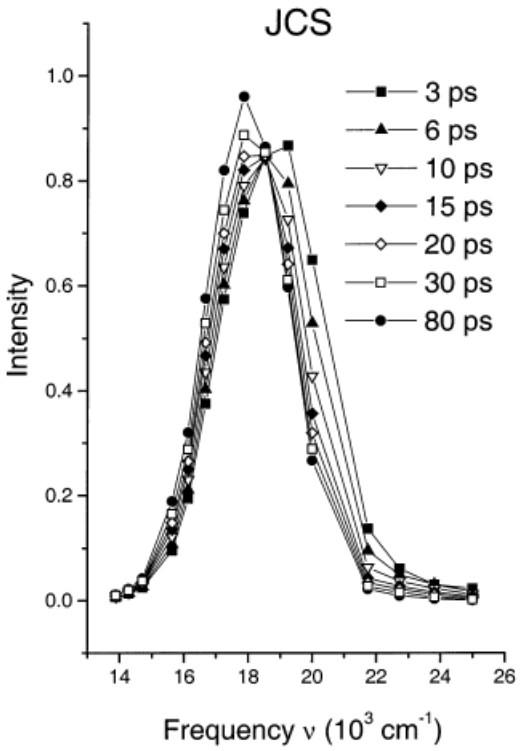
Supporting Information

A. Comparison of two evolutions of JCS fluorescence presented in ref. 13.

B. DCS crystal structure

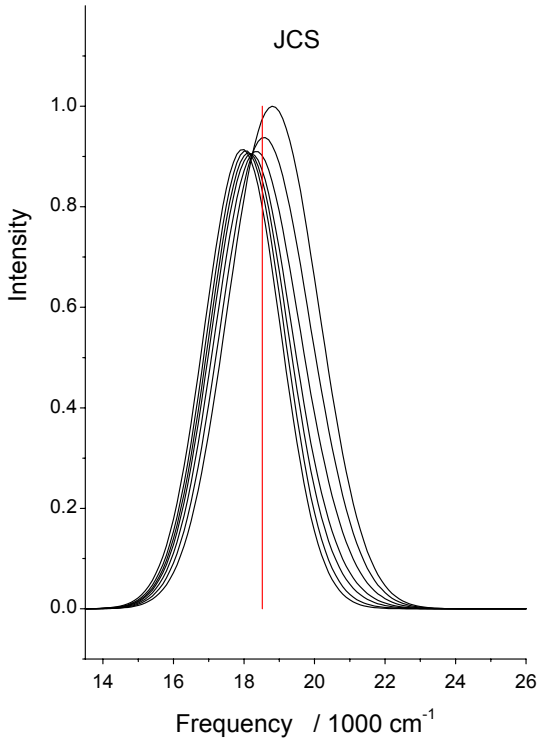
C. JCS crystal structure

A. Comparison of two evolutions of JCS fluorescence presented in ref. 13.



left: **Fig. 2 in ref [13]**.

"Time-resolved emission spectra of JCS in ethanol at 298 K reconstructed from emission decay curves. An isoemissive point is observed at 540 nm (18520 cm^{-1})."

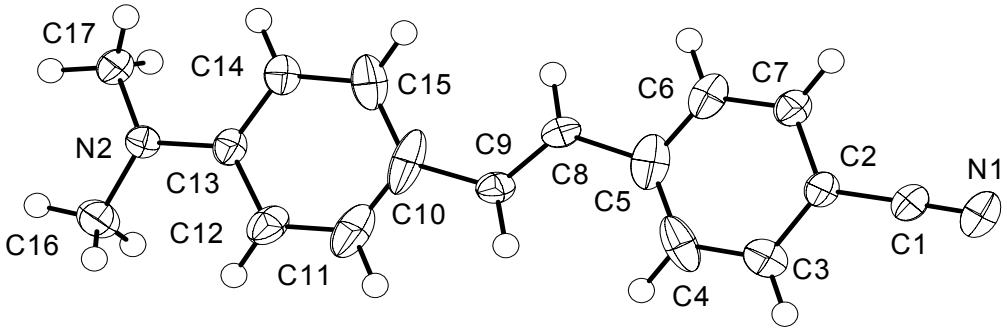


left:

Data given in the Supporting Information to ref. 13 result in the simulated JCS fluorescence spectra shown here. Delay times are 3, 6, 10, 15, 20, 30, 80 ps as above. The red line marks 18520 cm^{-1}. Comparison with the figure above shows that ref. 13 is not consistent regarding the JCS data which are discussed there.

B. DCS crystal structure

[CAS Registry number 2844-17-9]

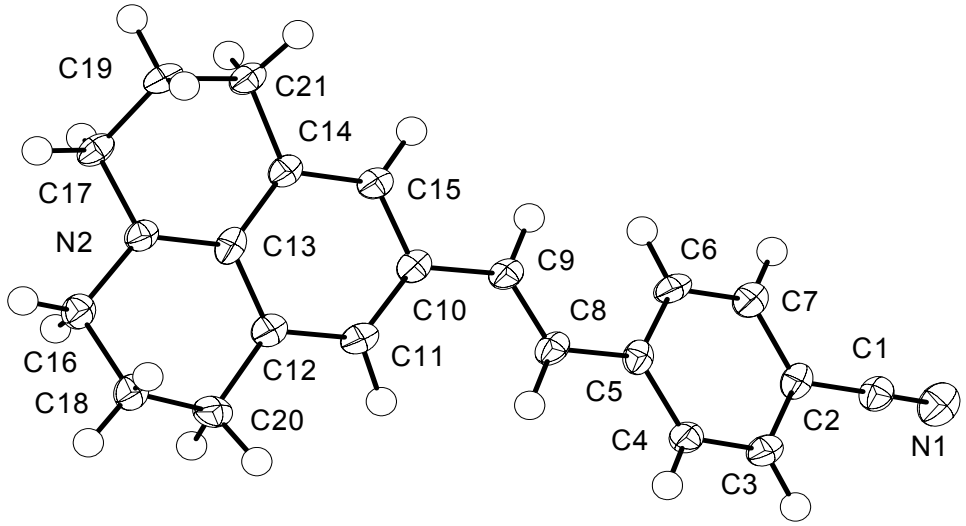


Atomic coordinates [Å] on the molecular principal axes:

N1	7.76237	0.00853	-0.27154
C1	6.61947	0.00939	-0.16110
C2	5.18557	0.01683	-0.04152
C3	4.40034	0.03531	-1.18984
C4	3.01301	0.04055	-1.04887
C5	2.39704	0.03414	0.21059
C6	3.21581	0.01944	1.31028
C7	4.58303	0.01710	1.21362
H3	4.80063	0.04418	-2.05133
H4	2.4699	0.04868	-1.82827
H6	2.81966	0.01051	2.17369
H7	5.117	0.01567	1.99934
C8	0.92227	0.04594	0.58770
C9	0.00223	-0.03432	-0.36118
H8	0.66325	0.11059	1.49941
H9	0.27932	-0.06769	-1.26926
C10	-1.43845	-0.07349	-0.05234
C11	-2.19128	-0.06453	-1.20159
C12	-3.54854	-0.0689	-1.19851
C13	-4.27492	-0.10338	-0.00382
C14	-3.54667	-0.13158	1.18895
C15	-2.15533	-0.11683	1.16325
H11	-1.74058	-0.05481	-2.03782
H12	-4.01524	-0.04809	-2.02573
H14	-4.00377	-0.16093	2.02124
H15	-1.6763	-0.13643	1.98343
N2	-5.65827	-0.13343	-0.01706
C16	-6.35626	0.14827	-1.26133
C17	-6.38732	0.25282	1.16928
H16	-6.0811	-0.4988	-1.94397
H16	-6.13502	1.05437	-1.56208
H16	-7.32304	0.07909	-1.11648
H17	-7.34483	0.09809	1.02913
H17	-6.23334	1.20317	1.35238
H17	-6.07822	-0.28085	1.93088

C. JCS crystal structure

[CAS registry number 228579-67-7]



Atomic coordinates [Å] on the molecular principal axes:

N1	8.5537	-0.53277	0.2751
C1	7.43571	-0.33898	0.17687
C2	6.01145	-0.10385	0.03671
C3	5.48324	0.33412	-1.18198
C4	4.1135	0.50076	-1.29794
C5	3.24579	0.25469	-0.23443
C6	3.8046	-0.15861	0.98298
C7	5.16036	-0.33649	1.12045
H3	6.06788	0.46617	-1.93516
H4	3.79384	0.81771	-2.13667
H6	3.2389	-0.32684	1.76103
H7	5.55205	-0.70099	1.98383
C8	1.80054	0.37342	-0.43281
C9	0.86785	0.33428	0.51506
H8	1.5636	0.46337	-1.37798
H9	1.09729	0.27641	1.44688
C10	-0.57911	0.27314	0.31179
C11	-1.1703	0.16545	-0.94284
C12	-2.53839	0.002	-1.11806
C13	-3.38036	-0.03894	0.01105
C14	-2.81294	0.10961	1.29964
C15	-1.43457	0.2597	1.4104
H11	-0.61831	0.12224	-1.79622
H15	-1.06667	0.36358	2.30459
N2	-4.76227	-0.14677	-0.13875
C16	-5.28106	-0.62901	-1.41401
C17	-5.5419	-0.52818	1.03674
H16	-6.29273	-0.43383	-1.48921
H16	-5.05083	-1.65548	-1.5787
H17	-6.55476	-0.35478	0.78429
H17	-5.3262	-1.42976	1.32485
C18	-4.59879	0.11605	-2.55451

C19	-5.14248	0.34652	2.20043
H18	-4.96268	-0.20005	-3.40732
H18	-4.88473	1.07378	-2.42591
H19	-5.70859	0.14526	3.00707
H19	-5.29749	1.3122	1.99862
C20	-3.10697	-0.1632	-2.50679
C21	-3.67041	0.0866	2.54123
H20	-2.57339	0.43799	-3.19182
H20	-2.86507	-1.06088	-2.93788
H21	-3.38495	0.80376	3.25677
H21	-3.51366	-0.91389	2.99136