Electronic Supporting Information

An nπ* gated decay mediates excited-state lifetimes of isolated azaindoles

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ESI1. Formation of 7-AI homoclusters

7-AI forms very stable homodimers (7-AI_2, binding energy>20 kcal mol^{-1}) which can interfere in the detection of the isolated monomer, especially when ionization based detection schemes are employed. The formed dimers can fragment during the ionization, since they will be detected in the monomer mass-channel. To avoid the formation of the dimers and/or minimize their contribution to the monomer mass-channel signal, a fine tuning of the experimental conditions, particularly those related to the expansion as the stagnation pressure and the valve-laser timing, is required. In order to illustrate the influence of these parameters, mass-spectra and transients at the 7-AI monomer (118 Da) and 7-AI_2 dimer (236 Da) mass-channels were recorded at different valve-laser delays, following excitation and ionization at 289 and 800 nm, respectively (see Fig. ESI1a_i, b_i and c_i). Previously, the optimum conditions of heating temperature and carrier gas (Ar) pressure were established at 398 k and 1.5 atm, respectively. Figures SI5a_i exhibit measurements recorded in the presence of dimers in the expansion. The dimer mass-channel in Fig. ESI1a_3 shows the well-known dynamics that has been previously attributed to the dimer.[1-6] Additionally, the presence of a long-living background suggests the formation of bigger clusters. These features are considerably weaker, but still perceptible, in Fig. ESI1b_3. Simultaneously, the monomer mass-channels in Fig ESI1a_2 and ESI1b_2 show a rising component that can be attributed to the dynamics of fragmenting clusters. On the other hand, the data shown in Figures ESI1c_i were recorded at valve-laser delays that minimize the formation of clusters. At these conditions, the dimer channel does not show any meaningful signal, while the decays of the monomer channel can be safely assigned to the isolated 7-AI molecule.

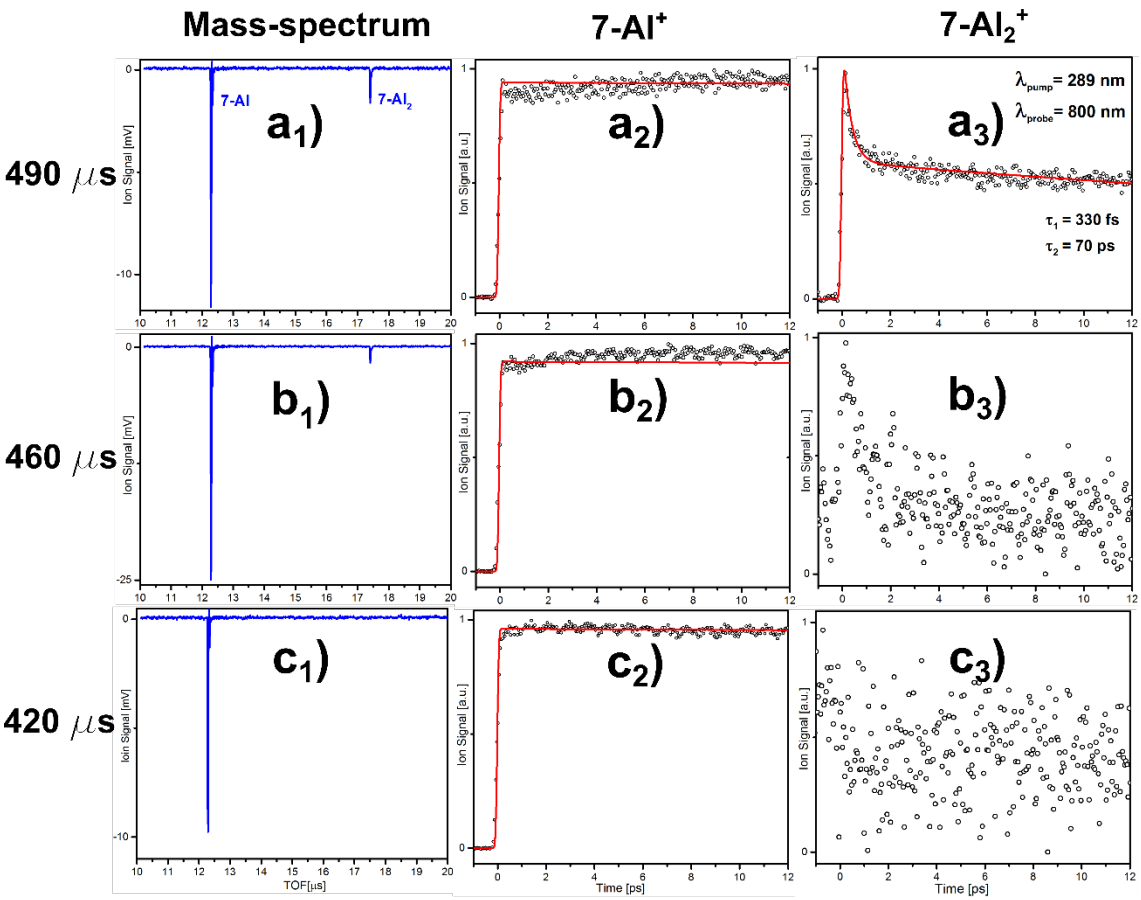


Figure ESI1. Mass spectra (a_1, b_1 and c_1) and decays recorded at the 7-Al^+ (a_2, b_2 and c_2) and 7-Al_2+ (a_3, b_3 and c_3) mass channels, at three different valve-pump delays: 9.51 (a_i), 9.54 (b_i) and 9.58 ms (c_i). The pump and probe wavelengths were 289 and 800 nm, respectively, for all the experiments.

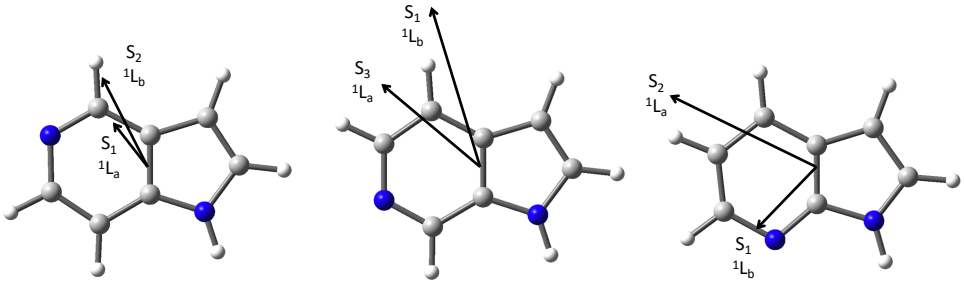
ESI2. Comparison of vertical excitation spectrum of 7-AI calculated in this work with previous theoretical estimates.

Table ESI1.

	S_1			S_2			S_3		
	E_{rel} [eV]	f	θ [°]	E_{rel} [eV]	f	θ [°]	E_{rel} [eV]	f	θ [°]
MS-CASPT2/ ANO-L[a]	4.69	0.043	45	4.77	0.081	-26	5.33	0.008	-
EOM-CCSD/ aug-cc-pvtz[b]	4.85 (pp*)	-	-	5.19 (pp*)	-	-	5.40 (np*)	-	-
B2PLYP/ 6-311+g(2d,p)[c]	5.09	0.042	-	4.96	0.187	-	5.66	0.003	-
SACCI/cc-pvtz[d]	4.03	0.094	28	4.23	0.159	-	4.61	0.005	-
CASPT2/ANO[e]	4.22	0.043	27	4.49	0.072	-29	5.27	0.008	-
CASPT2/ 6-31g(d,p)[f]	4.43	0.049	30	4.95	0.069	-34			-

[a]This work. [b]Ref. 7. [c]Ref. 8; basis set includes Rydberg [2s,2p] diffuse functions on C,N atoms. [d]Ref. 8; cc-pvdz for H; basis set on C,N atoms includes [2s,2p,2d] diffuse functions. [e]Ref. 9. [f]Ref. 10.

ESI3. Calculated excitation polarization



(a) 5-AI (b) 6-AI (c) 7-AI

Figure ESI2. Calculated polarization at the FC geometry for the lowest ππ* states at the MS-CASPT2/ANO-L level of theory for (a) 5-AI, (b) 6-AI and (c) 7-AI. The states more aligned along the horizontal (long) axis are labeled ^1L_a, and those along the vertical (short) axis ^1L_b.

ESI4. TD-CAM-B3LYP/6-311G* energies of critical points of 5-, 6- and 7-AI.

Table ESI2.

	5-AI E_{S1} [eV][a,b]		6-AI E_{S1} [eV][a,b]		7-AI E_{S1} [eV][a,b]	
	TD-DFT	MS-CASPT2	TD-DFT	MS-CASPT2	TD-DFT	MS-CASPT2
FC	5.25 (0.107)[c]	4.95 (0.028)	5.07 (0.080)	4.69 (0.083)	5.08 (0.084)	4.69 (0.043)
ππ*-Min	4.88 (0.130)	4.52 (0.137)	4.84 (0.117)	4.29 (0.141)	4.67 (0.124)[d]	4.26 (0.152)[b]
nπ*-Min	4.47 (0.003)	4.38 (0.006)	4.48 (0.014)	4.27 (0.027)	4.81 (0.049)	4.34 (0.081)
TS	4.64 (0.003)	4.38 (0.006)	4.57 (0.001)	4.34 (0.022)	4.91 (0.013)	4.60 (0.037)
S_1/S_0-CI[e]	4.55 (-)	3.92 (-)	4.61 (-)	4.17 (-)	4.60 (-)	4.15 (-)

[a]Oscillator strength in brackets. [b]Structures optimized at the TD-DFT level. [c]The lowest ππ* state is S_2 at the TD-DFT level. Energy and oscillator strength of S_1: 5.16 (0.002). [d]Additional ππ* minimum at 4.93 eV (oscillator strength 0.112). [e]CI optimized with the Tamm-Dancoff approximation. S_1/S_0 gaps at the full TD-DFT level: 0.11 (5-AI), 0.14 (6-AI) and 0.11 eV (7-AI).

ESI5. TD-DFT energy profiles

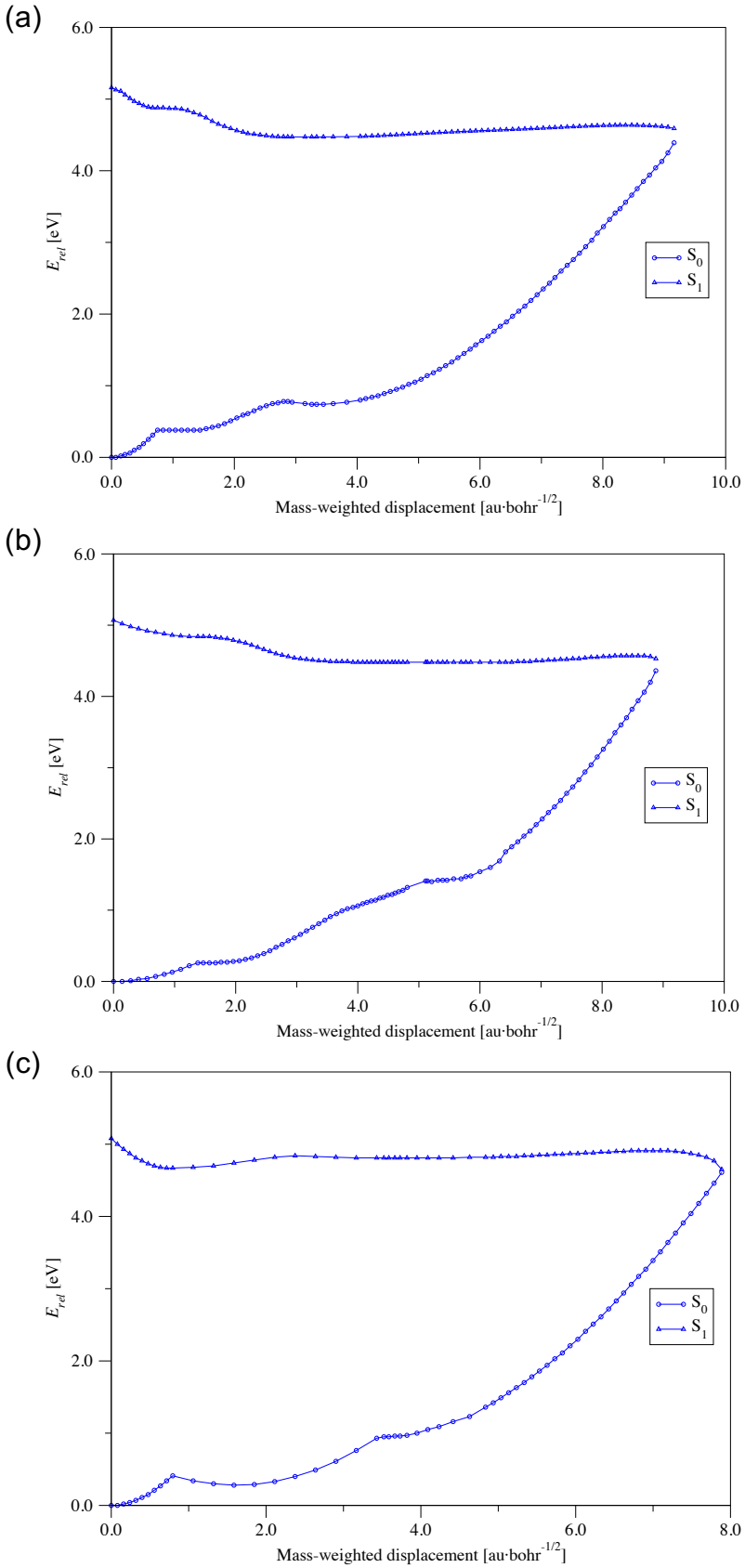


Figure ESI3. TD-CAM-B3LYP/6-311g** decay paths from the FC geometry to the lowest-energy CI for (a) 5-AI, (b) 6-AI and (c) 7-AI.

ESI6. Calculated structures for critical points along the relaxation pathways

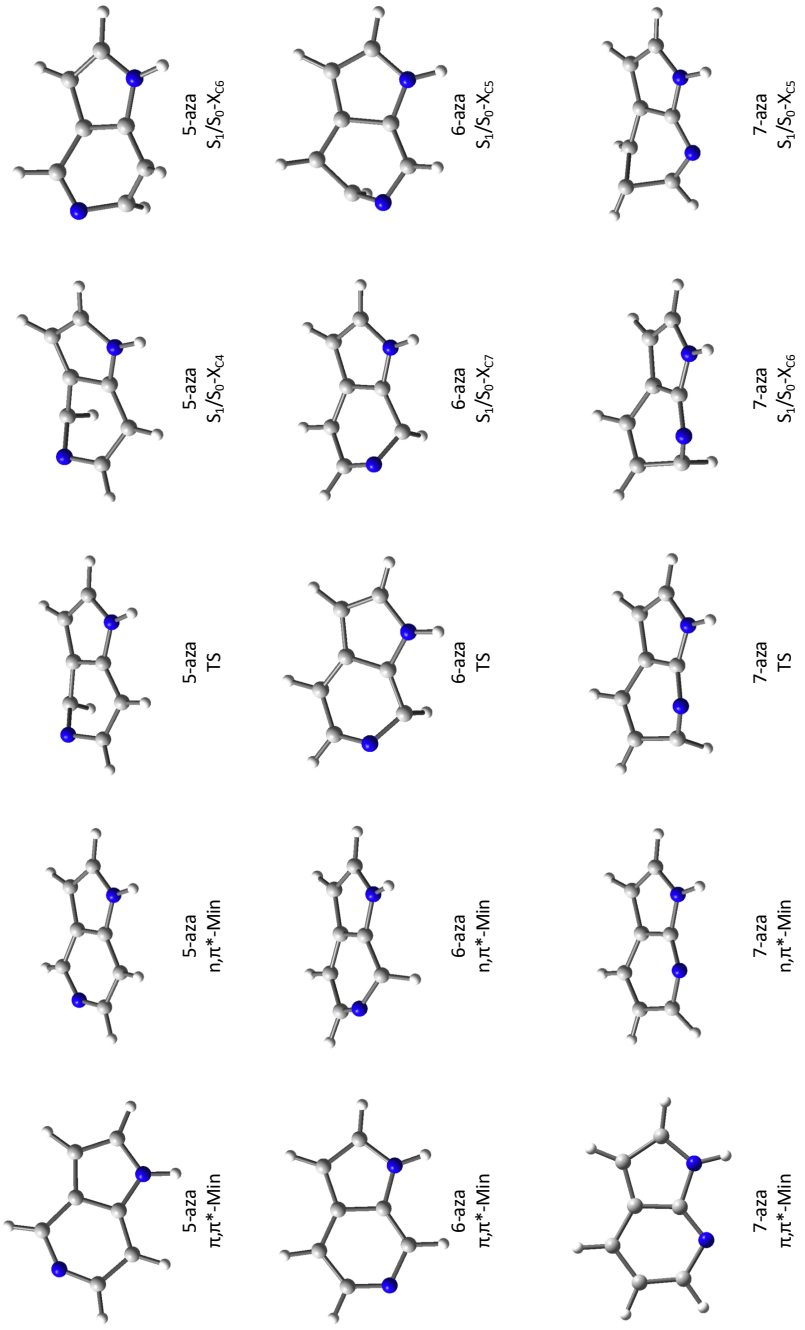


Figure ESI4. TD-CAM-B3LYP/6-311G** optimized structures for all compounds.

ESI7. Time-resolved ionization of 5-AI with the 400 nm probe

To test the possibility of ionizing from alternative locations as triplet states, time-resolved ionization measurements we carried out for 5-AI by using 400 nm radiation as ionizing probe (1+2'). The transients, shown in Figure ESI5, do not exhibit significant differences with those obtained with the 800 nm probe.

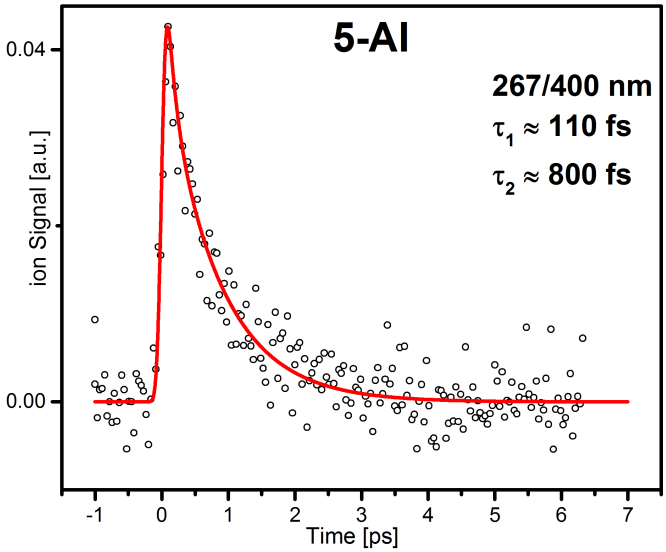


Figure ESI5. 5-AI$^+$ signals recorded at the 267 nm excitation wavelength, using 400 nm radiation as probe (1+2').

ESI8. NMe-7-AI time-resolved ionization

Aiming to confirm the observations made for the 7-AI monomer, especially the absence of dynamics due to dimers and bigger homoclusters, time-resolved ionization measurements were conducted on NMe-7-AI. The methyl group precludes the formation of clusters sustained by of N-H···N hydrogen-bonds. Figure ESI6 shows a one-color REMPI spectrum of jet-cooled NMe-7-AI recorded by a Nd:YAG pumped dye laser in the region of the electronic origin (~33238 cm^{-1}). The transients recorded after exciting at several vibronic bands across the spectrum and probing with 800 nm radiation are shown at long and short time-scales in Figures ESI7 and ESI8. The measured τ_1 between 400 and 200 fs and τ_2 that shortens from hundreds to tens of ps, perfectly match the dynamical behavior found for the 7-AI monomer.

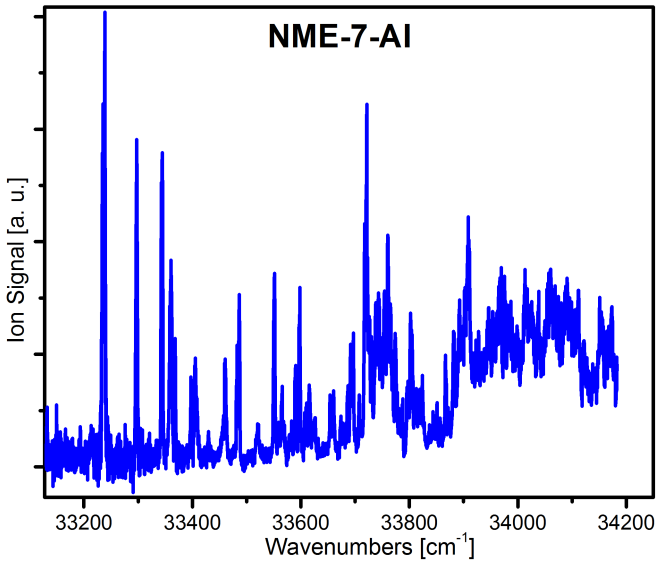


Figure ESI6. NMe-7-AI REMPI (1+1) spectrum.

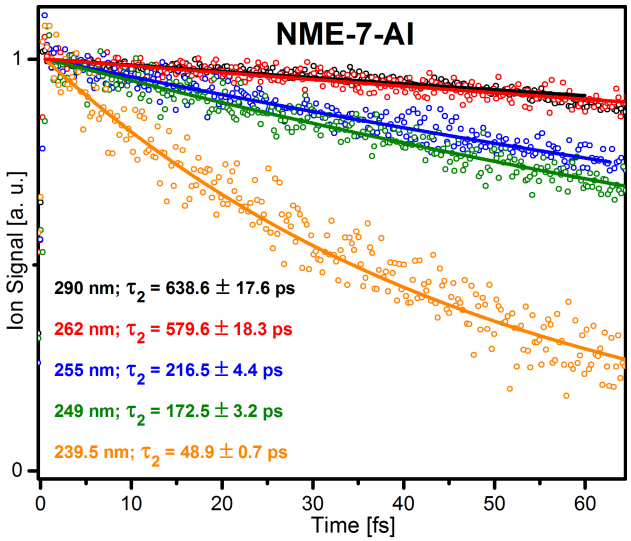


Figure ESI7. Long-scale transients recorded at the NMe-7-AI$^+$ mass-channel after exciting at the indicated wavelengths and probing with 800 nm radiation.

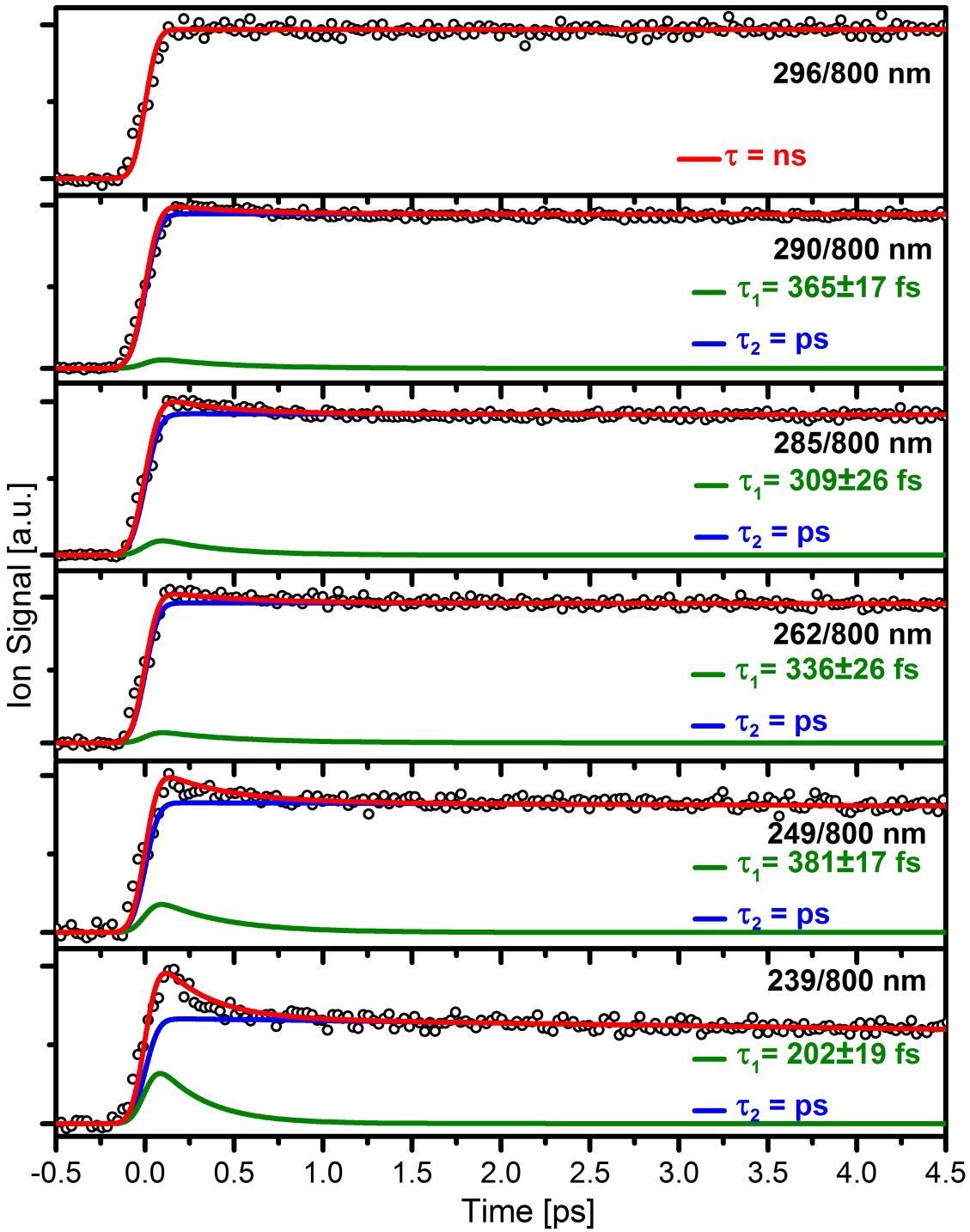


Figure ESI8. Short-scale transients recorded at the NMe-7-AI$^+$ mass-channel after exciting at the indicated wavelengths and probing with 800 nm radiation. The dots are the experimental values, the red line the best obtained fit and the green and blue lines the indicated temporal components deived from the fit.

ESI8. L_a/L_b crossing for 7-AI

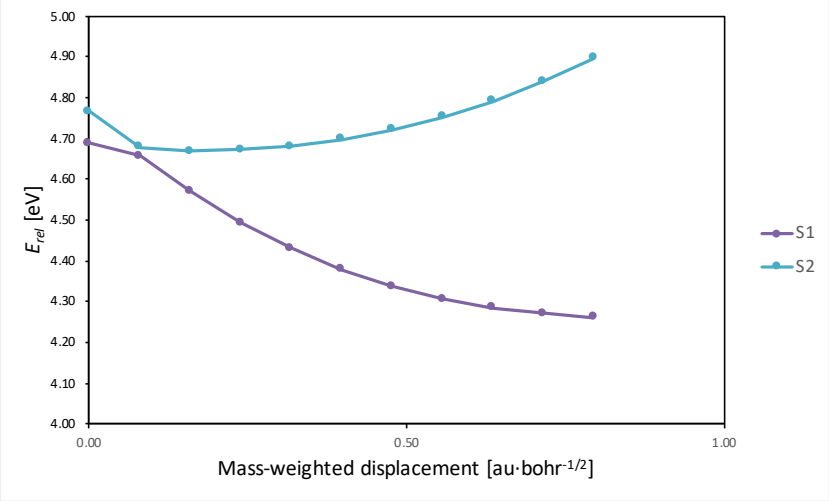


Figure ESI9. MS-CASPT2/ANO-L energy profile of the S_1 and S_2 states along the linear interpolation in internal coordinates between the FC structure and the lowest ππ* minimum for 7-AI, showing the L_a/L_b crossing.

ESI10. Steady-state fluorescence emission spectra in non-polar medium

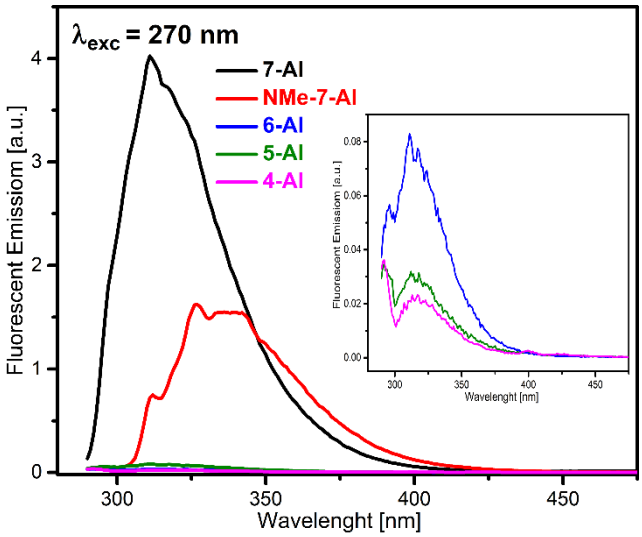


Figure ESI10. Steady-state fluorescence emission spectra of 3 x 10^{-5} M solutions of 4-, 5-, 6-, 7- and NMe-7-in cyclohexane, recoded in all cases at analogous conditions by exciting at 270 nm. The inset shows the 4-, 5- and 6-AI weaker emission spectra plotted on an expanded vertical scale.

ESI11. References

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ESI12. Cartesian coordinates of (TD)-CAM-B3LYP optimized structures

5-AI FC

C	-0.6725	-0.2464	0.0000
C	0.7364	-0.2423	0.0000
C	1.3775	0.9992	0.0000
C	0.0360	-2.3712	0.0000
C	1.1622	-1.6129	0.0000
H	2.4624	1.0625	0.0000
H	-2.0310	-1.8703	0.0000
H	-0.0770	-3.4435	0.0000
H	2.1751	-1.9813	0.0000
N	-1.0777	-1.5529	0.0000
C	-1.3838	0.9513	0.0000
H	-2.4660	0.9917	0.0000
N	0.7164	2.1421	0.0000
C	-0.6284	2.1049	0.0000
H	-1.1230	3.0709	0.0000

5-AI ππ*-Min

C	-0.6588	-0.2445	-0.0000
C	0.7430	-0.2375	-0.0000
C	1.4192	1.0111	0.0000
C	-0.0115	-2.4085	-0.0000
C	1.1572	-1.5824	-0.0000
H	2.4983	1.0827	0.0000
H	-2.0294	-1.8850	-0.0000
H	-0.1122	-3.4804	-0.0000
H	2.1684	-1.9591	-0.0000
N	-1.0659	-1.5853	-0.0000
C	-1.4045	0.9277	0.0000
H	-2.4836	0.9685	0.0000
N	0.7075	2.1844	0.0000
C	-0.6006	2.1273	0.0000
H	-1.1206	3.0828	0.0000

5-AI nπ*-Min

C	-0.6495	-0.2443	0.0102
C	0.7492	-0.2668	0.0329
C	1.4734	0.9972	0.0404
C	0.0285	-2.3897	-0.0027
C	1.1641	-1.6237	0.0168
H	2.5290	1.1413	-0.1143
H	-2.0225	-1.8358	-0.0347
H	-0.0976	-3.4589	0.0010
H	2.1764	-1.9943	0.0322
N	-1.0620	-1.5417	-0.0026
C	-1.4332	0.9506	-0.0225
H	-2.5054	0.9885	0.0827
N	0.6208	2.0175	0.0239
C	-0.6671	2.1341	0.0021
H	-1.0976	3.1278	0.0347

5-AI S_1-TS

C	-0.5628	-0.2438	-0.0231
C	0.8067	-0.3161	0.2343
C	1.4209	1.0074	0.0715
C	0.0204	-2.4010	0.0196
C	1.1719	-1.6819	0.2320
H	1.8599	1.2283	-0.9123
H	-1.9753	-1.7869	-0.3248
H	-0.1453	-3.4654	0.0008
H	2.1527	-2.0959	0.4012
N	-1.0214	-1.5222	-0.1445
C	-1.2521	1.0123	-0.2094
H	-2.3124	1.0534	-0.4225
N	0.6753	1.9621	0.6632
C	-0.5678	2.1484	0.1419
H	-1.0641	3.1033	0.2722

5-AI CI1

C	-0.4982	-0.2514	-0.2935
C	0.8570	-0.3354	0.0563
C	1.3744	1.0358	-0.0773
C	1.1545	-1.6776	0.3318
C	-0.0095	-2.3916	0.1195
H	1.4895	1.3440	-1.1231
H	-0.1949	-3.4495	0.2031
H	2.0979	-2.0925	0.6472
N	-1.0039	-1.5309	-0.2497
C	-1.1462	1.0130	-0.3158
H	-2.2096	1.0944	-0.5087
N	0.7748	1.9817	0.7046
C	-0.4742	2.1007	0.3132
H	-1.0534	2.9588	0.6481
H	-1.9517	-1.7975	-0.4557

5-AI CI2

C	0.8053	0.7858	-0.0044
C	0.0888	-0.4374	0.2577
C	-1.3206	-0.4237	-0.0243
C	1.0552	-1.4910	0.2507
C	2.2691	-0.9291	-0.0019
H	-1.8446	-1.3225	-0.3380
H	3.2428	-1.3879	-0.0710
H	0.8744	-2.5411	0.4175
N	2.1238	0.4325	-0.1735
C	0.1172	1.9819	-0.1961
H	0.3504	2.7567	-0.9111
N	-1.9302	0.7272	-0.0986
C	-1.1465	1.6717	0.4572
H	-1.2026	1.7315	1.5525
H	2.8735	1.0816	-0.3359

6-AI FC

C	-0.6361	-0.2644	0.0000
C	0.7718	-0.2204	0.0000
C	1.3717	1.0431	0.0000
C	0.5449	2.1455	0.0000
C	0.1214	-2.3663	0.0000
C	1.2312	-1.5763	0.0000
H	2.4480	1.1628	0.0000
H	0.9698	3.1437	0.0000
H	-1.9533	-1.9322	0.0000
H	0.0426	-3.4420	0.0000
H	2.2528	-1.9195	0.0000
N	-1.0096	-1.5877	0.0000
C	-1.3854	0.9092	0.0000
H	-2.4728	0.8913	0.0000
N	-0.8006	2.0916	0.0000

6-AI ππ*-Min

C	-0.6271	-0.2542	-0.0000
C	0.7861	-0.2294	-0.0000
C	1.3905	1.0411	0.0000
C	0.5147	2.1715	0.0000
C	1.2342	-1.5810	-0.0000
C	0.1073	-2.4162	-0.0000
H	2.4630	1.1801	0.0000
H	0.9692	3.1600	0.0000
H	0.0101	-3.4866	-0.0000
H	2.2580	-1.9217	-0.0000
N	-0.9871	-1.5852	-0.0000
C	-1.4000	0.8908	0.0000
H	-2.4828	0.8696	0.0000
N	-0.7971	2.1492	0.0000
H	-1.9429	-1.9096	-0.0000

6-AI nπ*-Min

C	-0.6610	-0.2883	0.1064
C	0.7365	-0.2202	0.0227
C	1.3698	1.0691	-0.0838
C	0.5647	2.1748	0.0592
C	0.1147	-2.3850	0.0100
C	1.2084	-1.5580	-0.0326
H	2.4445	1.1864	-0.0974
H	0.9584	3.1792	0.1618
H	-1.9556	-1.9492	0.2005
H	0.0474	-3.4600	-0.0001
H	2.2347	-1.8799	-0.1146
N	-1.0166	-1.6058	0.0919
C	-1.4801	0.8815	0.0243
H	-2.3400	0.9555	-0.6382
N	-0.7296	1.9779	0.2899

6-AI S_1-TS

C	-0.2929	-0.6925	-0.1005
C	-0.1968	0.6985	-0.0257
C	1.1183	1.2970	0.1463
C	2.2212	0.5024	-0.0056
C	-1.5234	1.1986	0.0112
C	-2.3677	0.1160	-0.0313
H	1.2330	2.3704	0.2231
H	3.2203	0.9058	-0.1209
H	-3.4438	0.0709	-0.0635
H	-1.8314	2.2305	0.0749
N	-1.6119	-1.0282	-0.0655
C	0.9378	-1.3871	0.2429
H	1.0603	-1.6646	1.3016
N	1.9624	-0.7863	-0.3937
H	-1.9711	-1.9644	-0.1495

6-AI CI1

C	-0.7204	-0.3629	0.1456
C	0.6244	-0.2357	-0.1786
C	1.1510	1.1053	-0.2797
C	0.4004	2.1714	0.2468
C	1.1625	-1.5584	-0.2017
C	0.1382	-2.4132	0.1006
H	2.2015	1.2636	-0.4922
H	0.8911	3.1048	0.5099
H	0.1294	-3.4844	0.2109
H	2.1766	-1.8495	-0.4267
N	-1.0127	-1.6744	0.2958
C	-1.3829	0.9397	-0.0311
H	-1.5357	1.1929	-1.0893
N	-0.8225	1.9244	0.7131
H	-1.9049	-2.0455	0.5766

6-AI CI2

C	-0.6455	-0.2863	-0.2865
C	0.7977	-0.2488	-0.1940
C	1.4058	1.0008	-0.2199
C	0.3678	1.8394	-0.8092
C	1.2124	-1.6067	0.0557
C	0.0947	-2.3791	0.0655
H	2.3543	1.2754	0.2138
H	0.2075	1.7914	-1.8978
H	0.0050	-3.4495	0.1687
H	2.2246	-1.9571	0.1738
N	-1.0249	-1.6039	-0.1191
C	-1.3845	0.8930	0.0214
H	-2.3626	0.8583	0.4938
N	-0.7442	2.0312	-0.0737
H	-1.9561	-1.9620	-0.2363

7-AI FC

C	-0.6211	-0.2178	0.0000
C	0.7930	-0.2268	0.0000
C	1.4212	1.0165	0.0000
C	0.6182	2.1422	0.0000
C	-0.7754	2.0084	0.0000
C	0.0601	-2.3466	0.0000
C	1.1990	-1.6015	0.0000
H	2.5017	1.1022	0.0000
H	1.0540	3.1329	0.0000
H	-1.4031	2.8938	0.0000
H	-2.0064	-1.8035	0.0000
H	-0.0602	-3.4182	0.0000
H	2.2061	-1.9857	0.0000
N	-1.0416	-1.5214	0.0000
N	-1.4125	0.8441	0.0000

7-AI ππ*-Min1

C	0.0000	0.6542	0.0000
C	0.4325	-0.6733	0.0000
C	-0.5506	-1.6972	0.0000
C	-1.8850	-1.2124	0.0000
C	-2.1673	0.1307	0.0000
C	1.8475	-0.6436	0.0000
C	2.2692	0.7262	0.0000
H	-0.3063	-2.7485	0.0000
H	-2.7126	-1.9112	0.0000
H	-3.1959	0.4715	0.0000
H	3.2599	1.1480	0.0000
H	2.5221	-1.4860	0.0000
N	1.1659	1.4663	0.0000
N	-1.2178	1.1542	0.0000
H	1.1190	2.4755	0.0000

7-AI ππ*-Min2

C	0.0000	0.6873	0.0000
C	0.4603	-0.6858	0.0000
C	-0.5185	-1.7039	-0.0000
C	-1.8487	-1.2255	-0.0000
C	-2.1675	0.1613	-0.0000
C	2.2665	0.6794	0.0000
C	1.8930	-0.6312	0.0000
H	-0.2798	-2.7563	-0.0000
H	-2.6742	-1.9270	-0.0000
H	-3.2100	0.4576	-0.0000
H	1.0473	2.4715	0.0000
H	3.2371	1.1440	0.0000
H	2.5635	-1.4759	0.0000
N	1.0932	1.4643	0.0000
N	-1.2639	1.1637	-0.0000

7-AI nπ*-Min

C	-0.6485	-0.2651	0.1055
C	0.7682	-0.2379	0.1043
C	1.4067	1.0481	-0.0054
C	0.6255	2.1828	0.0204
C	-0.7728	2.0816	0.1623
C	0.0479	-2.3842	-0.0222
C	1.1723	-1.5899	-0.0047
H	2.4862	1.1245	-0.0059
H	1.0753	3.1660	0.0952
H	-1.3527	2.8465	0.6667
H	-2.0179	-1.8588	0.0801
H	-0.0596	-3.4548	-0.0441
H	2.1874	-1.9413	-0.1069
N	-1.0602	-1.5592	0.0064
N	-1.3247	0.8604	-0.0517

7-AI S_1-TS

C	-0.0355	-0.0009	-0.0428
C	0.0006	-0.0445	1.3637
C	1.3010	0.0438	1.9993
C	2.4306	-0.0868	1.2569
C	2.1535	-0.4787	-0.1309
C	-1.3369	0.1524	1.7996
C	-2.1229	0.2845	0.6847
H	1.3639	0.1873	3.0728
H	3.4148	-0.1407	1.7051
H	2.3211	-1.5375	-0.3870
H	-3.1900	0.3998	0.5926
H	-1.6866	0.2041	2.8187
N	-1.3201	0.2259	-0.4353
N	1.1326	0.1766	-0.6946
H	-1.6317	0.2737	-1.3903

7-AI CI1

C	-0.7032	-0.2860	0.0224
C	0.7074	-0.2099	0.1443
C	1.1467	1.1808	0.1821
C	0.5877	2.0876	-0.7904
C	-0.5318	1.8913	0.0933
C	1.2030	-1.5197	0.1028
C	0.1077	-2.3541	-0.0411
H	1.9876	1.4833	0.7995
H	1.0128	3.0770	-0.9092
H	-0.8576	2.7213	0.7169
H	0.0756	-3.4293	-0.1098
H	2.2284	-1.8491	0.1488
N	-1.0463	-1.6134	-0.1024
N	-1.4050	0.8088	0.0496
H	-1.9799	-1.9701	-0.2068

7-Al Cl2

C	0.7504	0.7449	-0.0611
C	0.0669	-0.4789	0.2414
C	-1.3720	-0.4975	0.0473
C	-2.0042	0.6931	-0.0592
C	-1.0496	1.7414	0.3664
C	1.0576	-1.4922	0.2909
C	2.2644	-0.9011	0.0214
H	-1.8834	-1.4396	-0.1224
H	-3.0417	0.8217	-0.3334
H	-0.9646	1.8698	1.4538
H	3.2496	-1.3370	-0.0214
H	0.9099	-2.5424	0.4869
N	2.0805	0.4421	-0.2163
N	0.1036	1.8643	-0.3464
H	2.7984	1.1169	-0.4164