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Supplementary Materials

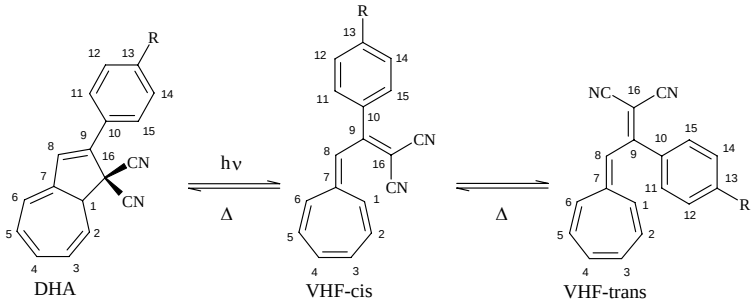

Table S1: Selected distances (Å) and angles (°) for the DHA form, as calculated at the B3LYP/6-311G* level of approximation.

DHA	R = H		R = CH_3		R = NH_2		R = NO_2	
	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN
C_1-C_2	1.509	1.509	1.509	1.510	1.508	1.509	1.509	1.508
C_2-C_3	1.345	1.346	1.345	1.346	1.346	1.347	1.345	1.346
C_3-C_4	1.446	1.448	1.446	1.447	1.445	1.447	1.446	1.448
C_4-C_5	1.360	1.361	1.360	1.361	1.364	1.361	1.361	1.360
C_5-C_6	1.438	1.439	1.437	1.439	1.437	1.438	1.437	1.438
C_6-C_7	1.357	1.358	1.357	1.358	1.358	1.360	1.358	1.358
C_1-C_7	1.518	1.520	1.518	1.519	1.516	1.520	1.518	1.521
C_7-C_8	1.436	1.436	1.435	1.435	1.436	1.433	1.434	1.434
C_8-C_9	1.353	1.354	1.353	1.354	1.355	1.359	1.354	1.357
C_9-C_{16}	1.553	1.553	1.553	1.554	1.557	1.554	1.553	1.550
C_1-C_{16}	1.597	1.596	1.597	1.598	1.596	1.595	1.598	1.594
C_9-C_{10}	1.465	1.465	1.464	1.464	1.458	1.455	1.463	1.461
C_{10}-C_{11}	1.410	1.411	1.410	1.410	1.410	1.414	1.411	1.412
C_{11}-C_{12}	1.387	1.388	1.385	1.387	1.381	1.380	1.383	1.383
C_{12}-C_{13}	1.396	1.397	1.402	1.402	1.408	1.413	1.393	1.395
C_{13}-C_{14}	1.391	1.393	1.396	1.398	1.404	1.409	1.388	1.391
C_{14}-C_{15}	1.391	1.393	1.390	1.391	1.385	1.385	1.388	1.388
C_{10}-C_{15}	1.406	1.407	1.404	1.407	1.408	1.410	1.408	1.401
C_8-C_9-C_{16}	108.7	108.4	108.7	108.6	108.7	108.1	108.9	108.5
C_7-C_8-C_9-C_{16}	-5.4	-5.8	-4.8	-5.0	1.7	-5.7	-4.5	-6.0
C_7-C_8-C_9-C_{10}	176.6	177.5	176.9	177.3	-178.0	178.0	177.4	178.4
C_8-C_9-C_{10}-C_{11}	-12.7	-13.8	-10.5	-11.2	14.7	-11.0	-9.6	-17.0

Table S2: Selected distances (Å) and angles (°) for the VHF-*cis* form, as calculated at the B3LYP/6-311G* level of approximation.

VHF-cis	R = H		R = CH_3		R = NH_2		R = NO_2	
	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN
C_1-C_2	1.360	1.368	1.360	1.368	1.359	1.366	1.362	1.370
C_2-C_3	1.432	1.425	1.432	1.425	1.433	1.428	1.430	1.422
C_3-C_4	1.360	1.367	1.359	1.367	1.359	1.364	1.361	1.368
C_4-C_5	1.432	1.425	1.432	1.425	1.433	1.428	1.430	1.422
C_5-C_6	1.361	1.368	1.361	1.368	1.360	1.366	1.362	1.370
C_6-C_7	1.450	1.442	1.450	1.442	1.452	1.445	1.447	1.438
C_1-C_7	1.449	1.441	1.449	1.441	1.451	1.444	1.447	1.437
C_7-C_8	1.389	1.406	1.389	1.406	1.386	1.401	1.393	1.413
C_8-C_9	1.432	1.413	1.433	1.412	1.437	1.421	1.428	1.405
C_9-C_{16}	1.389	1.405	1.389	1.406	1.391	1.407	1.390	1.405
C_9-C_{10}	1.497	1.498	1.496	1.497	1.490	1.488	1.499	1.503
C_{10}-C_{11}	1.401	1.401	1.400	1.400	1.403	1.406	1.401	1.400
C_{11}-C_{12}	1.392	1.394	1.391	1.393	1.386	1.386	1.389	1.390
C_{12}-C_{13}	1.393	1.395	1.398	1.399	1.405	1.409	1.390	1.392
C_{13}-C_{14}	1.393	1.394	1.398	1.400	1.404	1.408	1.389	1.392
C_{14}-C_{15}	1.392	1.394	1.390	1.392	1.386	1.387	1.389	1.390
C_{10}-C_{15}	1.399	1.401	1.399	1.400	1.402	1.405	1.400	1.400
C_8-C_9-C_{16}	126.2	126.7	126.0	126.7	125.1	125.3	127.0	128.3
C_7-C_8-C_9-C_{16}	-33.7	-29.4	-34.4	-28.7	-35.9	-31.8	-32.2	-25.9
C_7-C_8-C_9-C_{10}	149.9	154.4	149.1	155.2	147.2	151.6	151.5	158.7
C_8-C_9-C_{10}-C_{11}	61.1	62.4	59.1	63.4	52.3	51.1	64.6	87.5

Table S3: Selected distances (Å) and dihedral angles (°) for the VHF-*trans* form, as calculated at the B3LYP/6-311G* level of approximation.

VHF-trans	R = H		R = CH_3		R = NH_2		R = NO_2	
	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN	In vacuo	In CH_3CN
C_1-C_2	1.361	1.368	1.360	1.368	1.360	1.366	1.361	1.369
C_2-C_3	1.434	1.425	1.434	1.425	1.435	1.428	1.433	1.423
C_3-C_4	1.359	1.366	1.359	1.366	1.358	1.364	1.359	1.368
C_4-C_5	1.433	1.424	1.433	1.425	1.434	1.428	1.432	1.423
C_5-C_6	1.361	1.368	1.360	1.368	1.360	1.366	1.361	1.369
C_6-C_7	1.452	1.443	1.452	1.443	1.453	1.446	1.451	1.440
C_1-C_7	1.452	1.442	1.453	1.443	1.454	1.446	1.451	1.441
C_7-C_8	1.389	1.407	1.389	1.406	1.386	1.401	1.391	1.409
C_8-C_9	1.431	1.412	1.432	1.413	1.437	1.422	1.428	1.408
C_9-C_{16}	1.391	1.408	1.391	1.409	1.393	1.412	1.391	1.408
C_9-C_{10}	1.490	1.491	1.488	1.488	1.480	1.473	1.492	1.493
C_{10}-C_{11}	1.402	1.402	1.401	1.401	1.405	1.409	1.402	1.402
C_{11}-C_{12}	1.391	1.392	1.390	1.392	1.384	1.382	1.388	1.388
C_{12}-C_{13}	1.394	1.396	1.399	1.399	1.407	1.412	1.391	1.392
C_{13}-C_{14}	1.393	1.395	1.399	1.401	1.405	1.411	1.390	1.392
C_{14}-C_{15}	1.393	1.394	1.391	1.391	1.386	1.384	1.390	1.390
C_{10}-C_{15}	1.400	1.401	1.400	1.402	1.403	1.408	1.401	1.402
C_8-C_9-C_{16}	119.4	120.1	119.3	119.9	118.8	119.0	119.9	120.7
C_7-C_8-C_9-C_{16}	-163.8	-167.3	-162.8	-165.2	-158.5	-158.8	-165.5	-168.9
C_7-C_8-C_9-C_{10}	20.6	17.0	21.5	19.2	25.6	25.3	19.3	16.4
C_8-C_9-C_{10}-C_{11}	55.4	57.8	53.8	54.9	47.4	44.5	57.3	58.8