

–Supplementary Material–
***peri*-Acenoacenes Molecules: Tuning of
the Singlet and Triplet Excitation
Energies by Modifying their Radical
Character**

A. Omist^a, G. Ricci^b, A. Derradji^a, A.J. Pérez-Jiménez^a,
E. San-Fabián^a, Y. Olivier^b, and J. C. Sancho-García^{a*}

^a Department of Physical Chemistry,
University of Alicante,
E-03080 Alicante, Spain

^b Unité de Chimie Physique Théorique et Structurale
& Laboratoire de Physique du Solid,
Namur Institute of Structured Matter,
Université de Namur,
B-5000 Namur, Belgium

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*E-mail: jc.sancho@ua.es

Contents

1 Cartesian coordinates of all compounds	3
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1 Cartesian coordinates of all compounds

Table S1: Cartesian coordinates of (1)

C	-5.63112	2.50470	0.24064
C	-6.86706	1.95452	0.23744
C	-7.05496	0.53842	0.16587
C	-5.90332	-0.29602	0.09747
C	-4.61376	0.27295	0.10078
C	-4.45402	1.69568	0.17296
C	-3.18298	2.23589	0.17511
C	-2.18485	0.01192	0.03665
C	-3.47450	-0.55704	0.03342
C	-0.73217	1.96861	0.10991
C	0.37162	1.14810	0.04358
C	0.22757	-0.23650	-0.02658
C	-1.03342	-0.82264	-0.03132
C	-8.31588	-0.04772	0.16104
C	-8.45976	-1.43218	0.08964
C	-7.35610	-2.25280	0.02370
C	-6.05557	-1.71299	0.02583
C	-4.90525	-2.52005	-0.04047
C	-3.63418	-1.97973	-0.03841
C	-2.45713	-2.78884	-0.10558
C	-1.22116	-2.23866	-0.10222
H	1.36320	1.58093	0.04581
H	1.10507	-0.86837	-0.07823
C	-2.03261	1.42887	0.10841
H	-0.61109	3.04294	0.16416
H	-3.06342	3.31137	0.22963
H	-5.51140	3.57940	0.29518
H	-7.74525	2.58569	0.28946
H	-2.57684	-3.86356	-0.15986
H	-0.34292	-2.86979	-0.15384
H	-5.02476	-3.59554	-0.09477
H	-7.47750	-3.32702	-0.03148
H	-9.19341	0.58385	0.21552
H	-9.45151	-1.86467	0.08507

Table S2: Cartesian coordinates of (2)

C	-4.457967	2.346910	0.192449
C	-5.679427	1.768562	0.151043
C	-5.833157	0.346510	0.097318
C	-4.659689	-0.462472	0.088142
C	-3.387315	0.133560	0.131127
C	-3.260127	1.564558	0.184630
C	-2.006925	2.134045	0.226247
C	-0.829799	1.354299	0.218221
C	0.440259	1.922672	0.260146
C	1.599909	1.141654	0.251764
C	2.893425	1.709185	0.294084
C	4.011806	0.912734	0.284393
C	3.898602	-0.479811	0.232423
C	2.654132	-1.092321	0.189381
C	1.480664	-0.283340	0.198587
C	0.208289	-0.879377	0.155641
C	-0.951786	-0.075330	0.164882
C	-2.227240	-0.670487	0.121902
C	-7.077626	-0.265995	0.054199
C	-7.190831	-1.658539	0.002207
C	-6.072451	-2.454993	-0.007437
C	-4.778936	-1.887466	0.034948
C	-3.619285	-2.668487	0.026596
C	-2.349227	-2.100116	0.068567
C	-1.172100	-2.879863	0.060561
C	0.081102	-2.310375	0.102177
C	1.278942	-3.092726	0.094375
C	2.500402	-2.514375	0.135721
H	4.994095	1.365068	0.317267
H	4.790925	-1.092614	0.225470
H	2.989524	2.786595	0.334434
H	0.533912	3.001187	0.300459
H	-1.914461	3.212782	0.266534
H	-4.364654	3.424856	0.232783
H	-6.572987	2.379935	0.157928
H	-7.969948	0.346810	0.061128
H	-8.173119	-2.110871	-0.030723
H	-6.168552	-3.532403	-0.047791
H	-3.712940	-3.747002	-0.013692
H	-1.264565	-3.958602	0.020327
H	1.185628	-4.170676	0.054124
H	3.393962	-3.125748	0.128863

Table S3: Cartesian coordinates of (**3**)

C	-4.130735	2.767944	-0.388449
C	-5.330936	2.147915	-0.337249
C	-5.434075	0.723549	-0.238255
C	-4.231733	-0.042050	-0.194104
C	-2.982574	0.596454	-0.246920
C	-2.905820	2.029698	-0.346105
C	-1.674654	2.642399	-0.396752
C	-0.468722	1.907101	-0.354629
C	-0.541062	0.473246	-0.255734
C	-1.793126	-0.164407	-0.203153
C	0.775839	2.519805	-0.405242
C	1.970049	1.783600	-0.363122
C	1.898702	0.350357	-0.264521
C	0.646637	-0.287305	-0.212058
C	3.225937	2.394775	-0.413650
C	4.407303	1.656316	-0.371374
C	4.337312	0.228028	-0.273240
C	3.088149	-0.410508	-0.220858
C	5.683228	2.267321	-0.422005
C	6.826701	1.511761	-0.378254
C	6.761155	0.116540	-0.282445
C	5.539653	-0.537584	-0.229311
C	-6.655572	0.069473	-0.184431
C	-6.721115	-1.325688	-0.087779
C	-5.577642	-2.081242	-0.043916
C	-4.301721	-1.470289	-0.095255
C	-3.120355	-2.208754	-0.053046
C	-1.864471	-1.597624	-0.104192
C	-0.670262	-2.333849	-0.062364
C	0.574297	-1.721169	-0.113321
C	1.780227	-2.456497	-0.071660
C	3.011392	-1.843795	-0.122297
C	4.236304	-2.582075	-0.080505
C	5.436508	-1.962016	-0.131277
H	7.793308	1.996172	-0.418038
H	7.674422	-0.463616	-0.249119
H	5.741893	3.345593	-0.496137
H	4.180928	-3.660844	-0.006437
H	6.351290	-2.540210	-0.098221
H	3.281905	3.474020	-0.487881
H	1.726400	-3.536039	0.002506
H	0.830186	3.599125	-0.479659
H	-0.724610	-3.413174	0.011968
H	-1.620828	3.721906	-0.471439
H	-3.176322	-3.287973	0.021547
H	-4.075363	3.846656	-0.463342
H	-6.245720	2.726075	-0.370809
H	-5.636305	-3.159472	0.030835
H	-7.568840	0.649617	-0.217969
H	-7.687718	-1.810058	-0.047420

Table S4: Cartesian coordinates of (4)

C	-1.144300	0.990117	-0.038359
C	-2.369226	0.339368	-0.052979
C	-2.399848	-1.100032	-0.075082
C	-1.189389	-1.826773	-0.081388
C	0.042566	-1.151961	-0.066325
C	0.072691	0.288771	-0.044339
C	1.305643	0.938695	-0.029744
C	2.515399	0.235727	-0.035728
C	3.756400	0.884315	-0.021149
C	4.956062	0.178741	-0.027216
C	6.215287	0.827605	-0.012586
C	-3.596134	1.040527	-0.046973
C	-6.054394	1.094781	-0.055588
C	-7.236153	0.438652	-0.070389
C	-7.297706	-0.991395	-0.092760
C	-6.073458	-1.723337	-0.099161
C	-4.843783	-1.047568	-0.083883
C	-4.808805	0.390740	-0.061619
C	-3.631937	-1.774820	-0.090210
C	1.253023	-1.878706	-0.072649
C	2.485115	-1.203925	-0.057638
C	4.926636	-1.255427	-0.049034
C	6.150880	-1.987380	-0.055436
C	7.352774	-1.296756	-0.040434
C	7.378878	0.103629	-0.019124
C	-8.499594	-1.682022	-0.108274
C	-8.525686	-3.082404	-0.130052
C	-7.362091	-3.806371	-0.136530
C	-6.102872	-3.157503	-0.121388
C	-4.903209	-3.863064	-0.127361
C	-3.662214	-3.214474	-0.112380
C	-2.452462	-3.917432	-0.118233
C	-1.219514	-3.267512	-0.103416
C	-0.002529	-3.968858	-0.109233
C	1.222394	-3.318116	-0.094565
C	2.449294	-4.019284	-0.100394
C	3.661968	-3.369506	-0.085869
C	4.907551	-4.073562	-0.091716
C	6.089318	-3.417438	-0.077270
C	3.696958	-1.931187	-0.063984
H	-6.029950	2.177085	-0.038705
H	-8.167314	0.990990	-0.065444
H	-3.573470	2.123566	-0.030236
H	-1.121851	2.072956	-0.021771
H	1.329121	2.021447	-0.013231
H	3.781468	1.967083	-0.004650
H	6.243236	1.909495	0.003925
H	8.331580	0.616240	-0.007745
H	8.282288	-1.851454	-0.045305
H	-9.429116	-1.127338	-0.103401
H	-9.478385	-3.595010	-0.141868
H	-7.390026	-4.888255	-0.153377
H	-4.928264	-4.945829	-0.144087
H	-2.475931	-5.000185	-0.134806
H	-0.024976	-5.051700	-0.125708
H	2.426624	-5.102328	-0.116835
H	4.883093	-5.155874	-0.108138
H	7.020474	-3.969785	-0.082032

Table S5: Cartesian coordinates of (5)

C	-6.961874	2.045071	0.000000
C	-8.153240	1.368254	0.000001
C	-5.729198	1.346130	0.000000
C	-4.503134	2.002990	-0.000000
C	-3.287767	1.305000	-0.000001
C	-2.053117	1.958858	-0.000002
C	-0.843999	1.259785	-0.000002
C	0.395191	1.911765	-0.000002
C	1.599489	1.211907	-0.000001
C	2.844143	1.863080	-0.000001
C	4.041510	1.163255	-0.000000
C	5.295632	1.814346	0.000000
C	6.481122	1.116215	0.000000
C	7.753974	1.769593	0.000002
C	8.908409	1.066403	0.000002
C	-8.183185	-0.032485	0.000002
C	-7.010047	-0.770813	0.000001
C	-5.757167	-0.088766	0.000000
C	-4.555834	-0.813344	-0.000000
C	-3.315220	-0.135802	-0.000001
C	-2.111625	-0.859385	-0.000001
C	-0.871916	-0.182632	-0.000001
C	0.331115	-0.906161	-0.000002
C	1.571151	-0.229683	-0.000001
C	2.774182	-0.953217	-0.000001
C	4.013893	-0.276472	-0.000000
C	5.217485	-1.000068	-0.000000
C	6.458102	-0.322538	0.000000
C	7.659435	-1.047133	0.000000
C	8.912317	-0.365093	0.000001
C	-7.006137	-2.202316	0.000002
C	-5.851697	-2.905499	0.000001
C	-4.578844	-2.252111	0.000000
C	-3.393353	-2.950225	-0.000000
C	-2.139235	-2.299131	-0.000000
C	-0.941868	-2.998939	-0.000001
C	0.302779	-2.347772	-0.000001
C	1.507078	-3.047620	-0.000001
C	2.746264	-2.395654	-0.000001
C	3.955384	-3.094724	-0.000001
C	5.190029	-2.440885	-0.000000
C	6.405397	-3.138878	-0.000000
C	7.631458	-2.482038	0.000000
C	8.864135	-3.180985	0.000000
C	10.055500	-2.504176	0.000001
C	10.085456	-1.103432	0.000001
H	-9.084659	1.918711	0.000002
H	-9.134122	-0.549596	0.000003
H	-6.946529	3.127335	0.000000
H	-4.484751	3.086014	-0.000001
H	-2.033069	3.041777	-0.000002
H	0.416363	2.994680	-0.000002
H	2.865645	2.946076	-0.000000
H	5.316640	2.897558	0.000000
H	7.773117	2.852138	0.000002
H	9.861019	1.580876	0.000002
H	11.036397	-0.586334	0.000002
H	8.848779	-4.263249	-0.000000
H	10.986920	-3.054633	0.000001
H	6.387004	-4.221902	-0.000001
H	3.935328	-4.177646	-0.000001
H	1.485900	-4.130538	-0.000001
H	-0.963372	-4.081936	-0.000000
H	-3.414357	-4.033437	0.000000
H	-5.870831	-3.988044	0.000002
H	-7.958747	-2.716792	0.000003

Table S6: Cartesian coordinates of (**6**)

C	-5.631729	2.463145	0.236136
C	-6.857304	1.908411	0.230769
C	-7.042970	0.494927	0.158913
N	-5.907933	-0.305142	0.093640
C	-4.629628	0.279428	0.099520
C	-4.478204	1.642094	0.169388
C	-3.161047	2.190468	0.172600
N	-2.187836	0.010979	0.036570
C	-3.466141	-0.573593	0.030746
C	-0.725298	1.953007	0.111584
C	0.362360	1.155527	0.047156
C	0.209080	-0.240771	-0.024691
C	-1.052804	-0.789076	-0.028944
C	-8.304855	-0.053380	0.154700
C	-8.458127	-1.449701	0.083250
C	-7.370463	-2.247195	0.019093
C	-6.040631	-1.704408	0.021536
C	-4.934719	-2.484640	-0.042199
C	-3.617565	-1.936257	-0.039159
C	-2.464046	-2.757293	-0.106207
C	-1.238475	-2.202551	-0.101000
H	1.353479	1.589706	0.050737
H	1.058355	-0.903872	-0.077176
C	-2.055134	1.410234	0.108878
H	-0.640878	3.028408	0.167619
H	-3.033561	3.261492	0.227468
H	-5.510767	3.537230	0.291142
H	-7.750592	2.514297	0.280856
H	-2.585010	-3.831372	-0.161329
H	-0.345192	-2.808422	-0.151342
H	-5.062201	-3.555676	-0.096855
H	-7.454875	-3.322616	-0.036555
H	-9.154134	0.609730	0.206989
H	-9.449243	-1.883887	0.079823

Table S7: Cartesian coordinates of (**7**)

C	-4.450814	2.310950	0.191307
C	-5.659615	1.731898	0.149960
C	-5.813841	0.310910	0.096248
N	-4.667570	-0.467688	0.087768
C	-3.395600	0.126034	0.130697
C	-3.268035	1.511510	0.182629
C	-1.995369	2.103537	0.225457
C	-0.845767	1.349614	0.217856
C	0.466356	1.896166	0.259724
C	1.584811	1.120856	0.250813
C	2.898343	1.685773	0.293346
C	4.007798	0.911959	0.284309
C	3.882750	-0.487009	0.231924
C	2.634819	-1.056717	0.190351
N	1.488545	-0.278124	0.198933
C	0.216574	-0.871851	0.156082
C	-0.955291	-0.064435	0.165215
C	-2.223735	-0.681383	0.121580
C	-7.061771	-0.258792	0.054595
C	-7.186822	-1.657763	0.002268
C	-6.077371	-2.431583	-0.006629
C	-4.763838	-1.866670	0.035961
C	-3.645387	-2.641986	0.027170
C	-2.333260	-2.095434	0.068999
C	-1.183658	-2.849358	0.061417
C	0.089008	-2.257328	0.104198
C	1.271790	-3.056765	0.095468
C	2.480593	-2.477706	0.136676
H	4.988619	1.367128	0.317252
H	4.746541	-1.133809	0.223278
H	2.962546	2.763562	0.333159
H	0.596273	2.968352	0.300455
H	-1.927881	3.183738	0.265415
H	-4.354690	3.388287	0.231709
H	-6.566795	2.319422	0.155703
H	-7.925561	0.388011	0.063176
H	-8.167643	-2.112930	-0.030728
H	-6.141576	-3.509375	-0.046384
H	-3.775306	-3.714175	-0.013494
H	-1.251146	-3.929561	0.021524
H	1.175667	-4.134104	0.055142
H	3.387774	-3.065227	0.130874

Table S8: Cartesian coordinates of (**8**)

C	-4.117579	2.738759	-0.385949
C	-5.303728	2.119774	-0.334438
C	-5.408240	0.694204	-0.235404
N	-4.237114	-0.046163	-0.193011
C	-2.984243	0.579456	-0.245175
C	-2.903667	1.980786	-0.342516
C	-1.666751	2.606389	-0.394613
C	-0.475309	1.890647	-0.353679
C	-0.549818	0.477892	-0.255529
C	-1.799171	-0.175016	-0.201576
C	0.792303	2.520587	-0.406294
C	1.953921	1.798742	-0.364624
C	1.905091	0.367778	-0.265297
C	0.655737	-0.285140	-0.211398
C	3.250487	2.375412	-0.413809
C	4.393391	1.636096	-0.370753
N	4.343033	0.238985	-0.273560
C	3.090167	-0.386667	-0.221524
C	5.686196	2.243886	-0.422147
C	6.821142	1.510769	-0.379216
C	6.738386	0.108400	-0.281198
C	5.514178	-0.501309	-0.230362
C	-6.632458	0.084507	-0.184581
C	-6.715236	-1.317934	-0.087691
C	-5.580307	-2.051129	-0.045563
C	-4.287499	-1.443336	-0.096586
C	-3.144594	-2.182677	-0.053864
C	-1.848017	-1.606023	-0.102661
C	-0.686383	-2.327862	-0.061100
C	0.581233	-1.697922	-0.113410
C	1.772698	-2.413620	-0.072344
C	3.009621	-1.788004	-0.124161
C	4.223547	-2.545905	-0.080060
C	5.409689	-1.926851	-0.130897
H	7.787087	1.995552	-0.419744
H	7.623971	-0.507647	-0.244582
H	5.714200	3.321503	-0.497259
H	4.163841	-3.623983	-0.005141
H	6.337199	-2.480903	-0.098832
H	3.351462	3.449292	-0.488962
H	0.836601	3.600342	-0.481337
H	-1.634993	3.686967	-0.469602
H	-4.057865	3.816831	-0.460926
H	-6.231223	2.673887	-0.365849
H	-5.608324	-3.128810	0.028623
H	-7.518034	0.700613	-0.220514
H	-7.681192	-1.802724	-0.047450
H	-3.245559	-3.256394	0.020662
H	-0.730740	-3.407416	0.013556
H	1.740933	-3.493989	0.002418

Table S9: Cartesian coordinates of (**9**)

C	-1.136985	0.972521	-0.045541
C	-2.372324	0.305270	-0.060917
C	-1.189131	-1.836637	-0.088632
C	0.034547	-1.149280	-0.072896
C	0.058834	0.284774	-0.050932
C	1.317153	0.943444	-0.035502
C	2.495417	0.252668	-0.040912
C	3.776310	0.863044	-0.026099
C	4.937571	0.151887	-0.031677
C	6.213151	0.796923	-0.016233
C	-3.591714	0.993891	-0.055560
C	-6.039675	1.060922	-0.064265
C	-7.206394	0.406280	-0.078708
C	-7.269213	-1.026280	-0.101249
N	-6.077555	-1.736642	-0.107629
C	-4.842464	-1.079800	-0.092431
C	-4.802381	0.337068	-0.070623
C	1.254768	-1.872510	-0.078635
C	2.491671	-1.186523	-0.062768
N	4.922950	-1.249253	-0.052908
C	6.114624	-1.959602	-0.058342
C	7.318702	-1.314578	-0.043226
C	7.367017	0.094665	-0.021696
C	-8.473278	-1.671308	-0.116191
C	-8.521609	-3.080546	-0.138578
C	-7.367755	-3.782808	-0.144945
C	-6.092173	-3.137767	-0.129514
C	-4.930918	-3.848928	-0.135677
C	-3.649997	-3.238558	-0.120719
C	-2.471780	-3.929368	-0.126295
C	-1.213432	-3.270743	-0.110714
C	-0.017663	-3.958496	-0.116023
C	1.217746	-3.291303	-0.100386
C	2.437138	-3.979830	-0.105356
C	3.647789	-3.322929	-0.089949
C	4.885086	-4.046797	-0.095309
C	6.051798	-3.392150	-0.080238
C	3.687903	-1.906117	-0.068345
H	-8.149864	0.933586	-0.073991
H	-6.010424	2.142677	-0.047466
H	-3.586509	2.077514	-0.039038
H	-1.127437	2.056112	-0.028954
H	1.335398	2.026534	-0.018952
H	3.850225	1.941788	-0.009518
H	6.211187	1.877463	0.000106
H	8.320404	0.604783	-0.009713
H	8.221231	-1.906931	-0.048140
H	4.855822	-5.128557	-0.111721
H	6.995276	-3.919454	-0.083978
H	2.432080	-5.063452	-0.121790
H	-0.027154	-5.042088	-0.132671
H	-2.490078	-5.012450	-0.143172
H	-5.004890	-4.927662	-0.152844
H	-9.375820	-1.078979	-0.110504
H	-9.475008	-3.590643	-0.150503
H	-7.365815	-4.863337	-0.161987
C	-3.646333	-1.799369	-0.098565
C	-2.409350	-1.113468	-0.082733

Table S10: Cartesian coordinates of (10)

C	-7.015668	2.035059	-0.049302
C	-8.195654	1.379387	-0.057455
C	-5.766163	1.340254	-0.046913
C	-4.579235	2.006516	-0.038518
C	-3.322639	1.347531	-0.036098
C	-2.119836	1.992170	-0.027812
C	-0.885592	1.286616	-0.025757
C	0.332383	1.923737	-0.017550
C	1.551550	1.212286	-0.015549
C	2.781580	1.855980	-0.007305
C	3.979752	1.141259	-0.005501
C	5.231112	1.782887	0.002843
C	6.409800	1.080595	0.004595
C	7.676250	1.753710	0.013186
C	8.815066	1.052451	0.014751
C	-8.200322	-0.032387	-0.063840
C	-7.024369	-0.724438	-0.061855
N	-5.804668	-0.061133	-0.053580
C	-3.378223	-0.092508	-0.043047
C	-2.164532	-0.825403	-0.041128
C	-0.924398	-0.152779	-0.032613
C	0.273000	-0.887285	-0.030821
C	1.522193	-0.219630	-0.022301
C	2.719606	-0.954140	-0.020596
C	3.959755	-0.281483	-0.012196
C	5.173458	-1.014384	-0.010439
C	6.392146	-0.343602	-0.002138
C	-7.019533	-2.159105	-0.068293
C	-5.880759	-2.860442	-0.066526
C	-4.614267	-2.187454	-0.058048
C	-3.435568	-2.889763	-0.056141
C	-2.184295	-2.248147	-0.047793
C	-0.986035	-2.962866	-0.045912
C	0.243903	-2.319245	-0.037603
C	1.463168	-3.030677	-0.035665
C	2.681073	-2.393593	-0.027469
C	3.915399	-3.099106	-0.025482
C	5.118155	-2.454442	-0.017369
C	6.374802	-3.113333	-0.015100
C	7.561739	-2.447128	-0.006977
C	8.811344	-3.142072	-0.004959
C	9.991182	-2.486182	0.003048
C	9.995606	-1.074415	0.009671
H	-9.128704	1.925672	-0.059129
H	-9.125248	-0.589247	-0.070229
H	-6.970982	3.114839	-0.044299
H	-4.612057	3.087485	-0.033611
H	-2.097084	3.075316	-0.022460
H	0.364537	3.007027	-0.012389
H	2.813572	2.939356	-0.002217
H	5.267582	2.866023	0.008030
H	7.690262	2.835833	0.018372
H	8.766443	-4.221833	-0.010168
H	10.924597	-3.031851	0.004399
H	6.407710	-4.194308	-0.020003
H	3.892876	-4.182259	-0.030642
H	1.431087	-4.113972	-0.040860
H	-1.018173	-4.046242	-0.051036
H	-3.472201	-3.972896	-0.061176
H	-5.895006	-3.942568	-0.071377
H	-7.983664	-2.647561	-0.074598
C	-4.596817	-0.763285	-0.051479
N	7.600037	-1.045720	-0.000281
C	8.819730	-0.382284	0.007984
H	9.779227	1.540816	0.021180
H	10.920716	-0.517845	0.016179