

Electronic Supporting Information

Electronic Structure and Vibrational Properties of

Indenotetracene-Based Crystal[†]

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Table S1. Converge criteria applied for the ground state optimizations of Monomer, Dimer 1, and Dimer 2 geometries at B3LYP/6-31+G(d,p) theory level.

<i>Threshold criteria</i>	Monomer	Dimer 1	Dimer 2
Max. Force: 0.000450 Hartree/Bohr	0.000011	0.000055	0.000005
RMS Force: 0.000300 Hartree/Bohr	0.000002	0.000007	0.000001
Max. Displacement: 0.001800 Bohr	0.000671	0.001067	0.000812
RMS Displacement: 0.001200 Bohr	0.000107	0.000159	0.000109

Table S2. Vertical Excitation Energies (in eV) and oscillator strengths (f, dimensionless) computed for singlet and triplet states at TD-CAM-B3LYP/6-31+G(d,p) level on the monomeric and dimeric structures optimized in the ground state at B3LYP/6-31+G(d,p) theory level.

E.S.	Monomer		Dimer 1		Dimer 2	
T1 _{Δ_{SCF}}	1.24	–	2.14	–	1.24	–
T1 _{stable}	1.24	–	1.24	–	1.24	–
T1 _{TDA}	1.25	–	1.25	–	1.25	–
S1	2.35	(0.258)	2.30	(0.010)	2.32	(0.000)
S2	2.64	(0.034)	2.34	(0.410)	2.35	(0.519)
S3	3.51	(0.055)	2.65	(0.033)	2.61	(0.053)
S4	3.58	(0.003)	2.67	(0.021)	2.62	(0.001)
S5	4.05	(0.040)	2.98	(0.001)	3.19	(0.000)
S6	4.21	(0.021)	3.21	(0.001)	3.20	(0.000)
S7	4.28	(0.065)	3.38	(0.003)	3.51	(0.003)
S8	4.48	(0.108)	3.38	(0.004)	3.51	(0.099)
S9	4.54	(0.940)	3.52	(0.002)	3.58	(0.002)
S10	4.59	(0.026)	3.52	(0.079)	3.58	(0.003)
S11	4.61	(0.151)	3.64	(0.000)	3.68	(0.001)
S12	4.75	(0.090)	3.88	(0.000)	3.68	(0.001)
S13	4.77	(0.346)	3.97	(0.000)	4.03	(0.002)
S14	4.80	(0.199)	4.03	(0.024)	4.04	(0.067)
S15	4.97	(0.039)	4.03	(0.039)	4.20	(0.046)
S16	5.00	(0.110)	4.16	(0.001)	4.20	(0.001)
S17	5.03	(0.105)	4.20	(0.012)	4.24	(0.000)
S18	5.06	(0.086)	4.20	(0.009)	4.25	(0.070)
S19	5.10	(0.061)	4.23	(0.022)	4.45	(0.265)
S20	5.15	(0.095)	4.23	(0.019)	4.45	(0.012)
S21	5.23	(0.003)	4.31	(0.021)	4.49	(0.007)
S22	5.30	(0.034)	4.31	(0.031)	4.50	(1.788)
S23	5.34	(0.125)	4.36	(0.002)	4.58	(0.003)
S24	5.36	(0.017)	4.46	(0.112)	4.58	(0.060)
S25	5.40	(0.011)	4.47	(0.027)	4.61	(0.011)
S26	5.47	(0.010)	4.48	(0.096)	4.63	(0.188)
S27	5.53	(0.051)	4.55	(1.346)	4.69	(0.000)
S28	5.56	(0.009)	4.59	(0.091)	4.71	(0.119)
S29	5.57	(0.004)	4.61	(0.223)	4.71	(0.028)
S30	5.61	(0.006)	4.72	(0.253)	4.76	(0.444)
S31	5.66	(0.053)	4.73	(0.045)	4.76	(0.000)
S32	5.66	(0.020)	4.75	(0.095)	4.77	(0.028)
S33	5.68	(0.030)	4.76	(0.164)	4.77	(0.007)
S34	5.72	(0.018)	4.77	(0.229)	4.78	(0.461)
S35	5.76	(0.005)	4.80	(0.278)	4.85	(0.009)
S36	5.78	(0.123)	4.82	(0.008)	4.86	(0.000)
S37	5.81	(0.018)	4.86	(0.044)	4.92	(0.005)
S38	5.83	(0.011)	4.87	(0.318)	4.93	(0.554)
S39	5.86	(0.005)	4.92	(0.015)	4.96	(0.000)
S40	5.89	(0.010)	4.94	(0.006)	4.96	(0.059)

Monomer

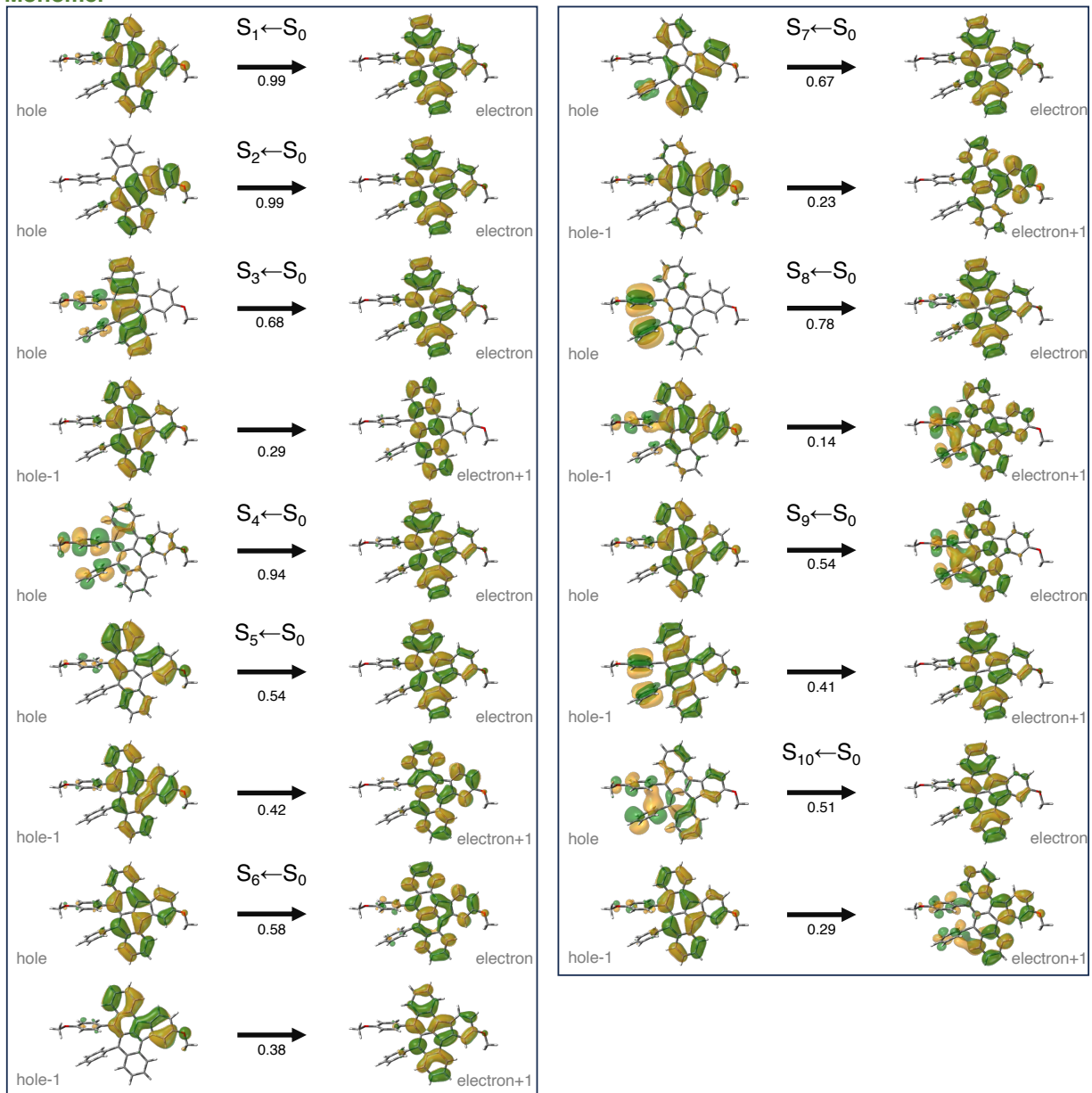


Figure S1. NTOs for the *hole-electron* transition of the first ten singlet excited states that contribute more than 20% calculated for Monomer case with the CAM-B3LYP functional. The iso-surface value=0.02 e/Bohr.

Dimer 1

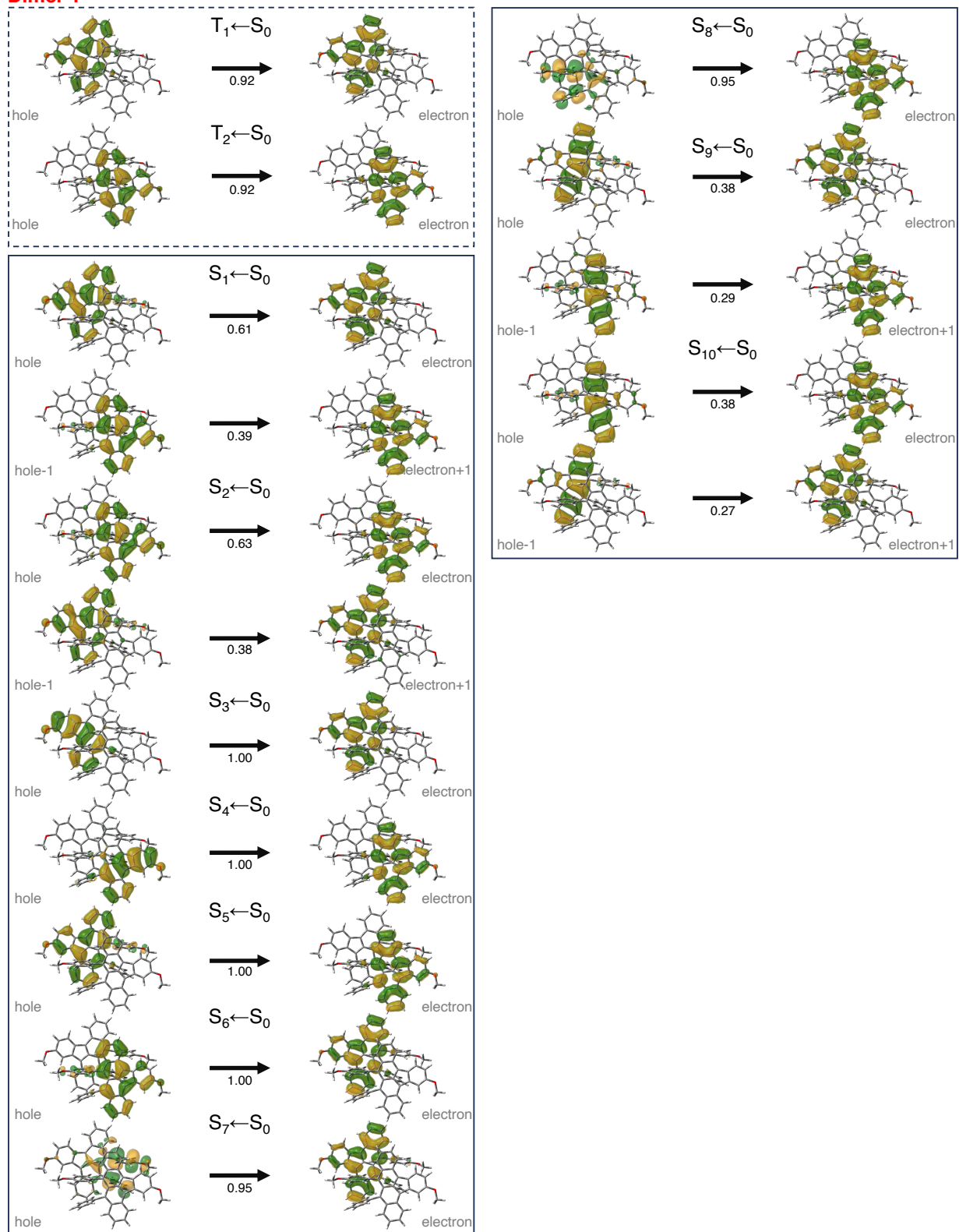


Figure S2. NTOs for the *hole-electron* transition of the first ten singlet excited states that contribute more than 20% calculated for Dimer 1 case with the CAM-B3LYP functional. The iso-surface value=0.02 e/Bohr.

Dimer 2

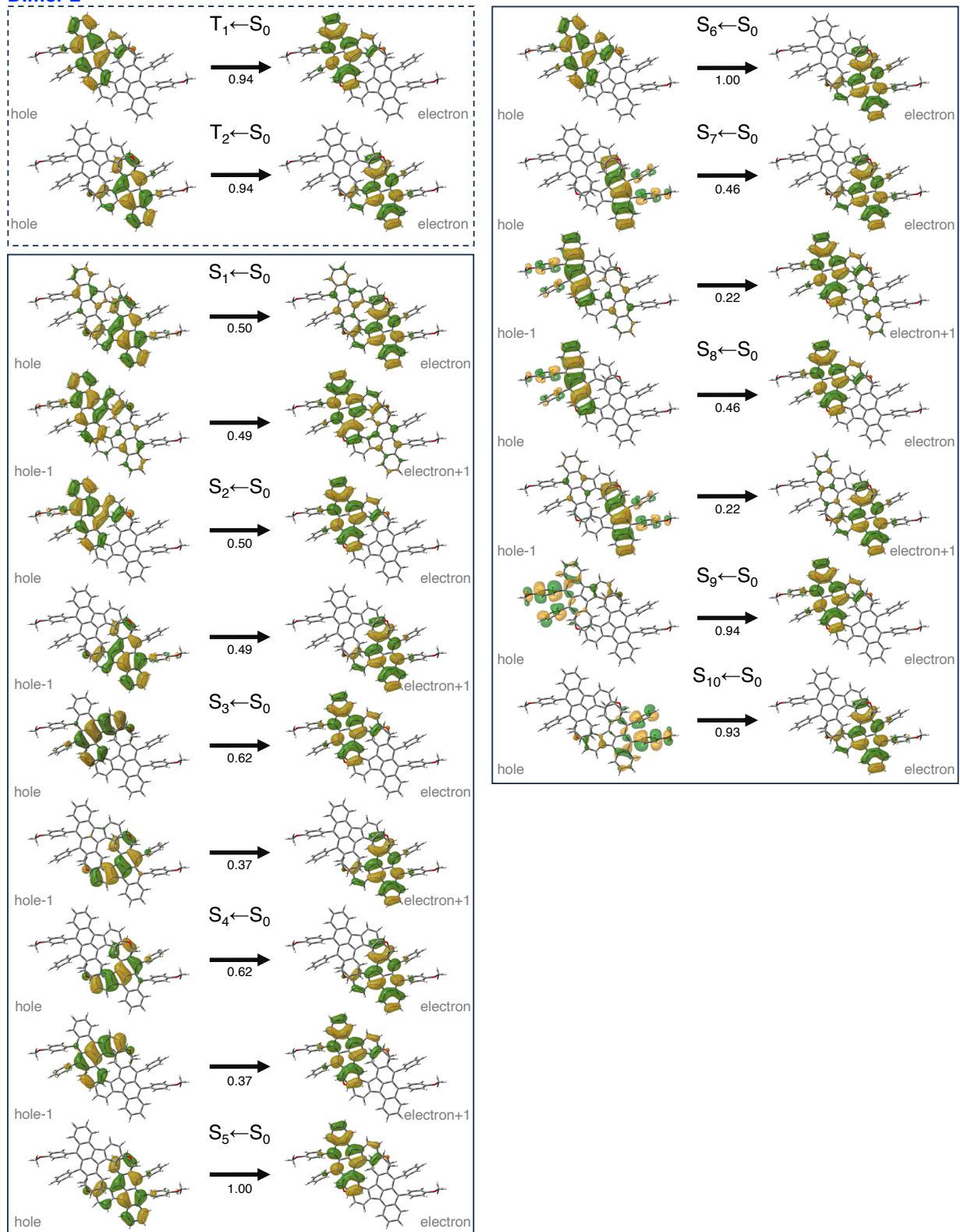


Figure S3. NTOs for the *hole-electron* transition of the first two triplet and first ten singlet excited states that contribute more than 20% calculated for Dimer 2 case with the CAM-B3LYP functional. The iso-surface value=0.02 e/Bohr.

Table S3. Ground to excited state transition electric dipole moments ($|d_{S_0-S_n}|^2$, in atomic units) and relative x , y , z components computed for the first ten singlet electronic states at TD-CAM-B3LYP/6-31+G(d,p) theory level for Dimer 1 and Dimer 2.

Dimer 1					Dimer 2				
E.S.	x	y	z	$ d_{S_0-S_n} ^2$	x	y	z	$ d_{S_0-S_n} ^2$	
S1	0.3981	0.1193	0.0502	0.1753	0.0095	-0.0017	0.0005	0.0001	
S2	2.4144	-1.0676	-0.4247	7.1495	2.6920	-1.2700	-0.3820	9.0057	
S3	-0.7012	-0.1316	-0.0058	0.5090	-0.3974	0.7784	0.2485	0.8256	
S4	0.1735	-0.5200	-0.1503	0.3231	-0.0512	0.0985	0.0310	0.0133	
S5	-0.0671	0.0652	-0.0284	0.0096	-0.0466	0.0065	-0.0083	0.0023	
S6	0.0021	0.0866	-0.0463	0.0097	0.0507	-0.0071	0.0090	0.0027	
S7	0.1326	-0.1231	-0.0891	0.0407	0.1395	0.1328	0.0413	0.0388	
S8	-0.1765	-0.1016	-0.0971	0.0509	0.7588	0.7285	0.2267	1.1580	
S9	0.1006	-0.0939	-0.0278	0.0197	-0.0438	0.1570	-0.0228	0.0271	
S10	-0.4580	-0.8282	-0.1360	0.9142	0.0540	-0.1787	0.0228	0.0354	

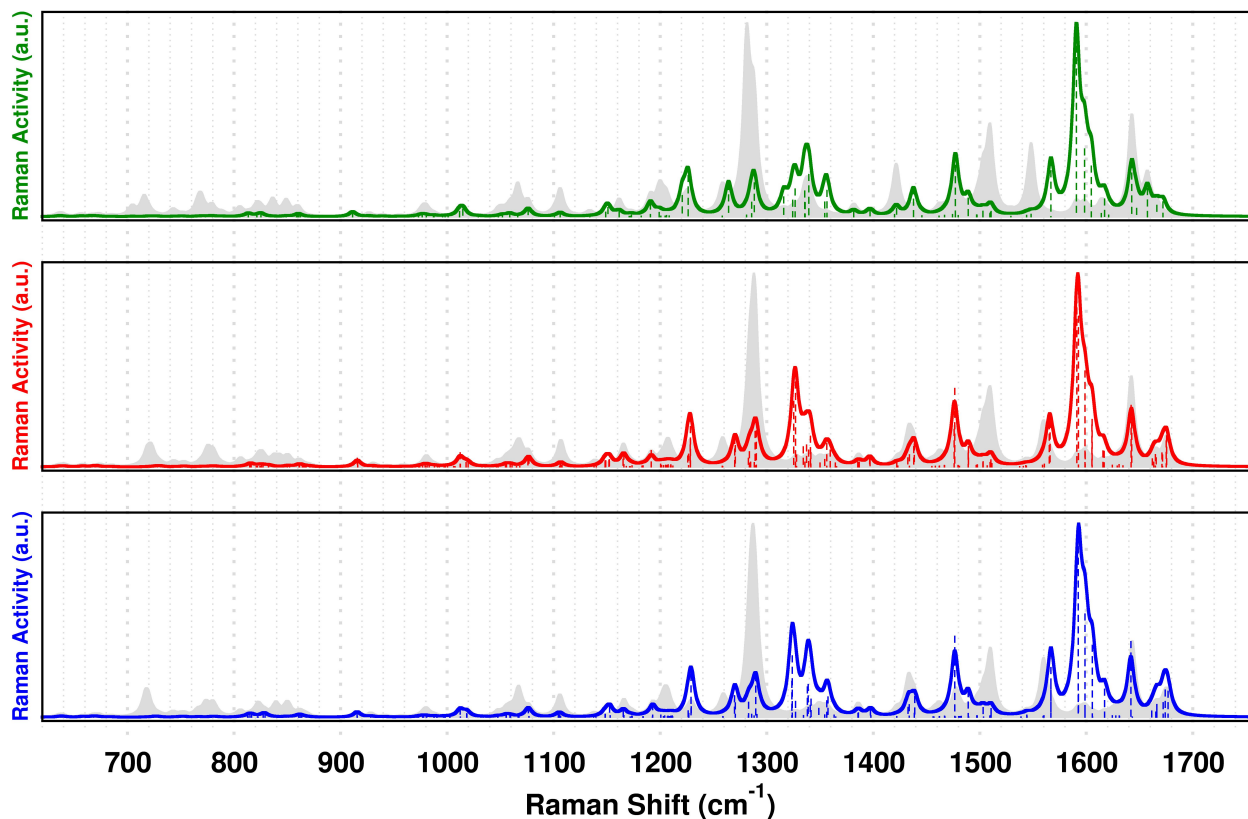


Figure S4. Infrared (gray) and Raman spectrum computed on the refined crystallographic structure of Monomer (top, green curve), Dimer 1 (center, red curve), and Dimer 2 (bottom, blue curve) in the ground state at B3LYP/6-31+G(d,p) theory level. Infrared intensity and Raman activity are reported in arbitrary units (a.u.) and normalized.

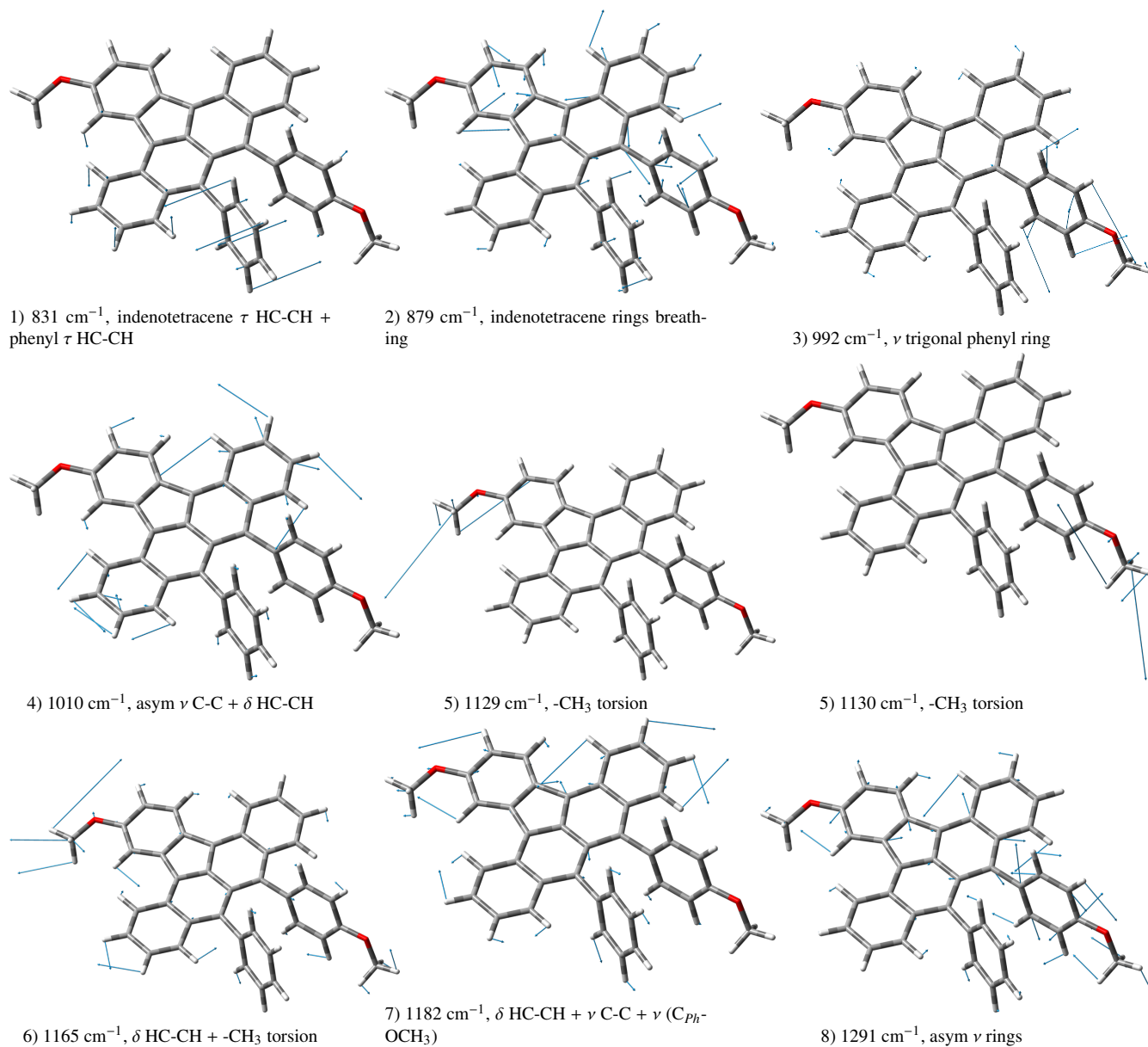


Figure S5. Normal modes displacement vectors computed at B3LYP/6-31+G(d,p) level associated to the Raman frequencies reported in Tab. 1. Descriptors for normal modes of vibration: τ twisting, δ scissoring, ρ rocking, ν stretching.

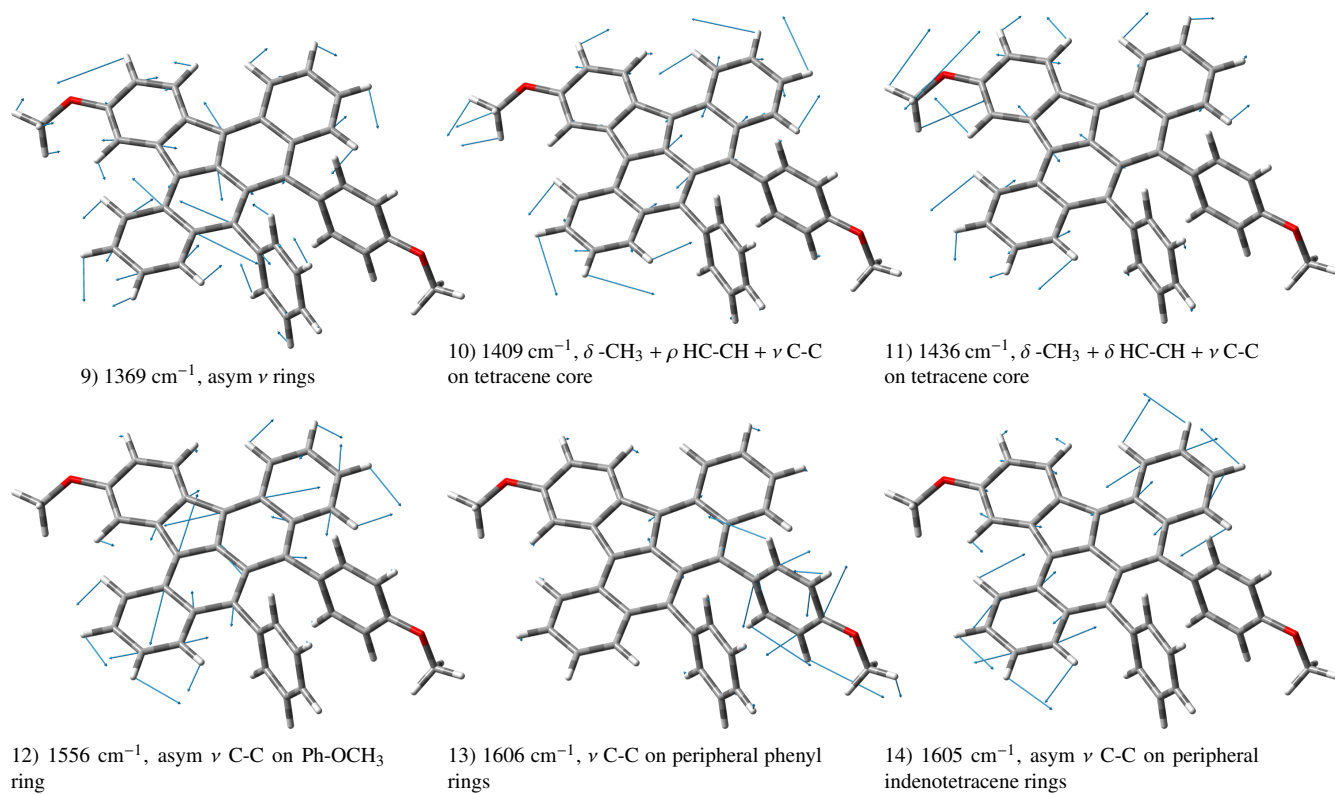


Figure S5. Normal modes displacement vectors computed at B3LYP/6-31+G(d,p) level associated to the Raman frequencies reported in Tab. 1 (*cont.*). Descriptors for normal modes of vibration: τ twisting, δ scissoring, ρ rocking, ν stretching.

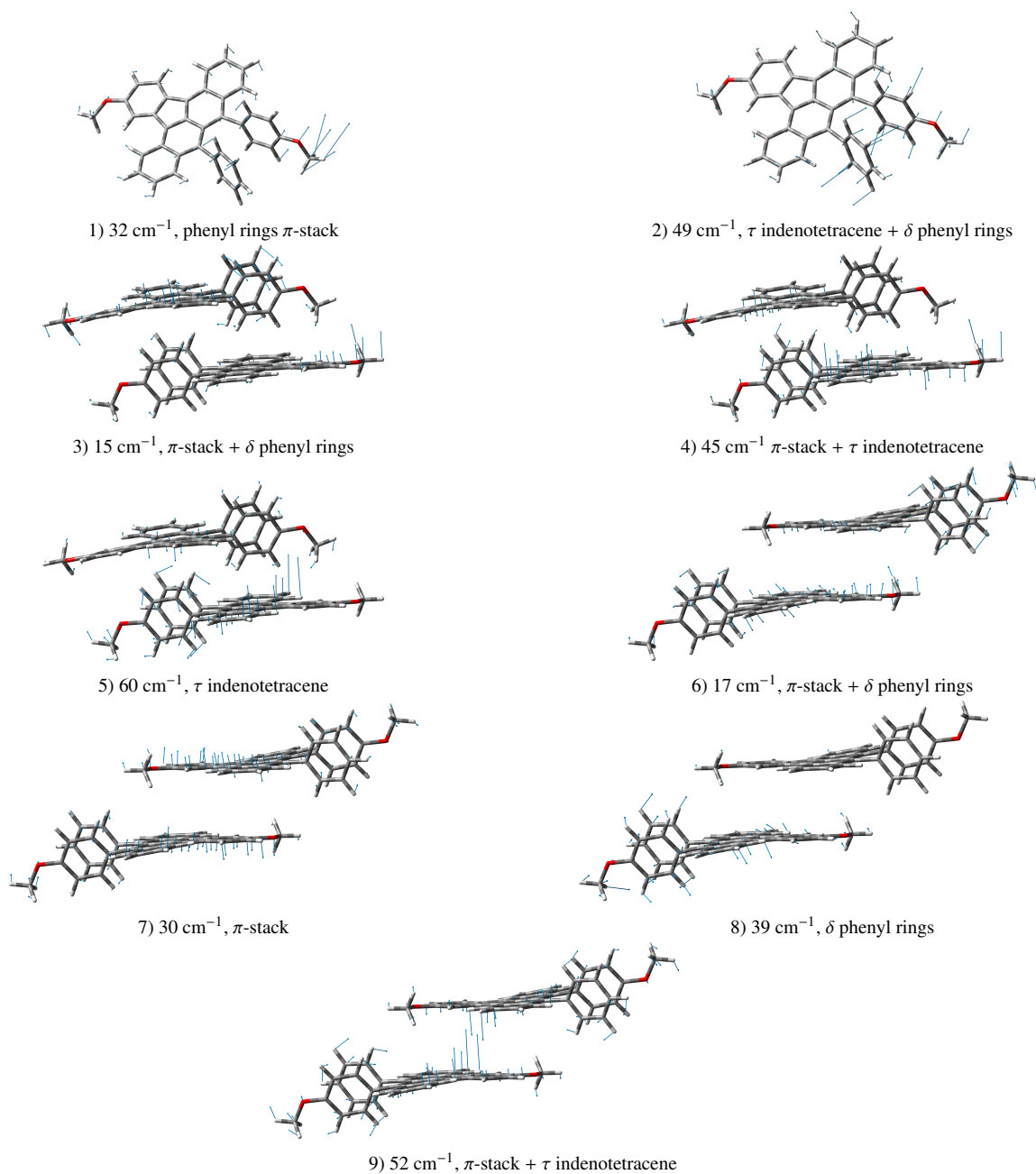


Figure S6. Normal modes displacement vectors computed at B3LYP/6-31+G(d,p) level associated to the Raman frequencies reported in Tab. 2.

S2 Equilibrium geometries in cartesian coordinates (Å) at B3LYP/6-31+G(d,p)

Table S4. Minimum energy structure of *DimethoxyASI* Monomer
(nuclear repulsion energy: 4200.8838590017 Hartrees)

C	1.19504	3.6804	0.12952	C	-0.15	-3.74751	0.16458
H	2.26754	3.55617	0.0571	H	0.89799	-4.00688	0.22463
C	0.67257	4.94396	0.19743	C	0.46597	-1.33596	0.07695
H	1.33472	5.80473	0.18174	C	3.09744	0.79883	-1.13702
C	-0.73603	5.13652	0.28656	H	2.52411	0.52617	-2.01782
H	-1.1409	6.14173	0.36128	C	-1.08042	-4.75158	0.18759
C	-1.57852	4.05754	0.26672	H	-0.75789	-5.78625	0.25708
H	-2.64532	4.21858	0.33232	C	-2.87899	-3.13874	0.07362
O	6.61702	1.20824	-0.06012	H	-3.93742	-2.92593	0.07544
C	0.36069	2.50632	0.14532	C	-2.3096	-0.70188	-0.00625
C	-3.3573	1.39493	0.01045	C	2.6259	-1.85744	1.28732
C	0.0861	0.04647	0.07984	C	-2.46829	-4.44323	0.14147
C	-3.61089	-0.00668	-0.05741	H	-3.20256	-5.24303	0.17653
C	2.42666	1.15238	0.03624	C	4.45096	-2.99168	0.16667
C	5.2501	1.16794	-0.09608	H	5.43749	-3.44538	0.19691
H	2.19702	-1.4393	2.19318	C	3.89847	-2.43315	1.32197
C	3.20812	1.50154	1.15427	C	7.33698	0.88826	-1.24399
H	2.71415	1.77508	2.08255	H	8.39209	0.99233	-0.98765
C	4.59607	1.51162	1.09662	H	7.09129	1.57918	-2.06042
H	5.19312	1.78065	1.96219	H	7.14081	-0.14187	-1.56653
H	4.45545	-2.44847	2.25449	C	2.45336	-2.38585	-1.05824
C	-1.31407	0.2989	0.05318	H	1.88386	-2.38227	-1.98373
C	-1.90037	1.58663	0.08784	C	3.72321	-2.96395	-1.0264
C	0.93083	1.20813	0.10458	H	4.14022	-3.39798	-1.93115
C	-1.08046	2.7171	0.17153	C	4.49422	0.81216	-1.21845
H	-4.29233	3.35759	-0.00989	H	4.9709	0.53639	-2.15151
C	-5.98419	0.42826	-0.22373	O	-7.30019	0.06742	-0.34126
C	-4.43689	2.28534	-0.04134	C	-4.92134	-0.48512	-0.18175
C	-5.74007	1.80667	-0.15202	H	-5.12543	-1.54155	-0.26374
H	-6.58399	2.48713	-0.19344	C	-7.62858	-1.3127	-0.42011
C	-0.52235	-2.35808	0.08127	H	-8.71552	-1.35522	-0.50138
C	-1.94416	-2.05295	0.03676	H	-7.3111	-1.853	0.48108
C	1.8863	-1.82353	0.09723	H	-7.18069	-1.78263	-1.30518

Table S5. Minimum energy structure of *DimethoxyASI* Dimer 1
(nuclear repulsion energy: 13441.0823277367 Hartrees)

C	7.373681	-0.768140	-0.999434	C	-8.508696	2.249555	0.560790
C	5.350653	-1.604670	-2.039854	H	-9.460044	2.755382	0.390125
C	6.707440	-1.741696	-1.756706	H	-8.354793	2.123717	1.640423
H	7.271894	-2.593218	-2.122115	H	-7.694759	2.855609	0.143017
C	6.682967	0.352742	-0.518314	O	3.781237	-5.151569	1.166085
O	8.706071	-0.998617	-0.783354	H	-8.659167	-1.251647	-1.257248
H	4.879238	-2.375199	-2.636301	O	-8.614316	0.995079	-0.098498
C	4.634767	-0.496068	-1.569337	H	-3.722222	3.110179	4.003900
C	5.316787	0.491648	-0.797893	H	3.774325	-1.525924	3.720009
H	7.216879	1.098821	0.049197	H	-6.858798	-2.921607	-1.348204
C	9.455997	-0.047009	-0.040273	C	-7.719143	-1.072896	-0.745997
C	3.235910	-0.065269	-1.719056	C	-7.549029	0.135291	-0.055949
C	4.341191	1.544459	-0.454061	H	-6.221452	1.354903	1.115235
H	9.071537	0.057270	0.982544	H	-4.939592	1.703154	2.426026
H	9.458950	0.934122	-0.532101	C	-3.228777	2.258197	3.544335
H	10.474782	-0.434893	-0.004016	C	2.762416	-1.475128	3.328743
C	2.141322	-0.584292	-2.419220	H	3.249703	-0.035792	1.804258
C	3.110956	1.169512	-1.039228	H	1.948716	-2.908412	4.724739
C	4.426225	2.719176	0.302243	H	-1.350638	2.568500	4.603160
C	2.187459	-1.794717	-3.184653	H	-4.825054	-6.496034	-2.302454
C	0.899081	0.175353	-2.383037	C	-6.692197	-2.013144	-0.783793
C	1.915524	1.938631	-0.971397	C	-6.347945	0.407444	0.613829
C	3.219372	3.521928	0.424507	C	-3.907913	1.471860	2.652026
C	5.613961	3.154613	0.975366	H	0.960629	0.113809	0.914773
C	1.096380	-2.245752	-3.878365	C	2.464397	-0.638314	2.251885
H	3.106937	-2.363041	-3.221305	H	-0.341250	-2.756538	3.815865
C	-0.210791	-0.343311	-3.139976	C	1.744286	-2.245623	3.888845
C	0.782229	1.396995	-1.669515	H	-0.241090	0.637718	3.620489
C	2.001796	3.153697	-0.213742	C	-1.882123	1.948982	3.886643
C	3.296927	4.702014	1.247025	H	-2.418471	-7.115035	-1.991068
H	6.513215	2.560047	0.903043	C	-4.164076	-5.834436	-1.749711
C	5.634496	4.296119	1.731906	H	-5.678776	-4.393469	-1.398077
C	-0.120936	-1.507075	-3.855760	C	-5.482403	-1.768226	-0.122132
H	1.158429	-3.166866	-4.450542	C	-5.320537	-0.544441	0.591611
H	-1.140051	0.211187	-3.147130	C	-3.298933	0.324207	2.047410
C	-0.515899	2.108349	-1.729853	C	1.172367	-0.551546	1.744491
C	0.861894	4.092502	0.004372	C	0.451558	-2.162795	3.369321
H	2.409009	5.303905	1.384343	C	-1.258634	0.863445	3.330318
C	4.455068	5.078931	1.873092	C	-2.797550	-6.191720	-1.562685
H	6.548077	4.597744	2.236418	H	-0.922976	-5.660831	-0.726018
H	-0.980183	-1.866827	-4.413635	C	-4.640434	-4.654487	-1.243846
C	-0.643829	3.241487	-2.522371	C	-4.221735	-2.520835	-0.018201
C	-1.648740	1.649632	-1.045695	C	-3.962274	-0.537739	1.167373
C	0.821504	5.329615	-0.651622	C	0.147421	-1.325565	2.298055
C	-0.104157	3.817649	0.974150	C	-1.924607	-0.004274	2.393106
H	4.470369	5.973132	2.489106	C	-3.796540	-3.759419	-0.508708
C	-1.853949	3.926979	-2.658586	C	-3.329127	-1.726323	0.739058
H	0.220827	3.602511	-3.071678	C	-1.268682	-1.151875	1.865938
H	-1.589724	0.762542	-0.424649	C	-1.959774	-5.376129	-0.849985
C	-2.847453	2.332943	-1.144861	C	-2.412511	-4.141393	-0.262982
H	1.581214	5.555179	-1.395745	C	-1.985177	-2.081478	1.041461
C	-0.151493	6.281494	-0.351121	H	0.674317	-2.345278	-0.698324
C	-1.083562	4.760423	1.264556	H	-0.615434	-5.392228	2.023490
H	-0.090394	2.872305	1.505792	C	-1.527923	-3.328369	0.492399
C	-2.968193	3.472095	-1.951075	C	-0.134610	-3.799359	0.658008
H	-1.900801	4.803538	-3.293386	H	2.992785	-3.067650	-0.423976
H	-3.724892	1.985414	-0.609966	C	0.180400	-4.888836	1.480799
C	-1.114902	5.997262	0.617556	H	1.731711	-6.171188	2.272154
H	-0.152222	7.236639	-0.869073	C	0.895109	-3.177933	-0.041007
H	-1.833875	4.526374	2.014356	C	2.210702	-3.593785	0.109636
O	-4.203468	4.061049	-1.975656	C	1.487793	-5.333077	1.627278
H	-1.881511	6.725373	0.866522	C	4.869608	-4.534348	0.487451
C	-4.394266	5.188836	-2.820032	H	5.764189	-5.064272	0.817368
H	-5.439552	5.477573	-2.701234	H	4.767780	-4.634406	-0.600284
H	-4.204666	4.937279	-3.871312	H	4.957083	-3.472945	0.744703
H	-3.749961	6.026162	-2.523827	C	2.519223	-4.673884	0.945641

Table S6. Minimum energy structure of *DimethoxyASI* Dimer 2
(nuclear repulsion energy: 12461.4161798055 Hartrees)

O	1.545646	-3.988804	-2.018531	H	1.929366	-4.081191	2.117432
C	-0.290851	-2.438760	-1.561742	C	7.549450	-3.866450	0.323881
H	0.284304	-1.600460	-1.921992	H	7.641224	-3.791555	2.481729
C	2.340223	-2.920316	-2.518110	H	-3.287780	3.371103	2.815385
H	3.286164	-3.372174	-2.819143	H	-2.529818	2.166059	1.741316
H	2.529302	-2.166901	-1.744405	H	-1.871760	2.446356	3.387218
H	1.869896	-2.447069	-3.389780	H	0.011233	-2.523078	2.519376
C	0.283096	-3.717970	-1.568033	O	11.063251	-1.227901	-0.617184
C	-1.600720	-2.275749	-1.094787	C	6.054390	2.785770	-0.325955
C	-0.441094	-4.824053	-1.102252	C	2.343285	3.399848	0.627442
C	-2.343407	-3.399911	-0.627700	C	4.882706	0.722253	0.381226
C	-2.480191	-1.090213	-1.011841	C	1.600582	2.275652	1.094448
C	-1.743815	-4.665672	-0.637189	C	7.371489	0.683304	-0.177395
H	0.030688	-5.800847	-1.123091	C	9.865519	-0.607560	-0.391838
C	-3.691206	-2.933001	-0.270740	H	5.656123	-1.793191	-1.610739
C	-3.732039	-1.543621	-0.539311	C	7.947123	0.450955	-1.433123
C	-2.306061	0.256782	-1.349651	H	7.430077	0.769372	-2.333641
H	-2.273441	-5.549744	-0.306534	C	9.164952	-0.194931	-1.533223
C	-4.839628	-3.579501	0.196982	H	9.612010	-0.390654	-2.503696
C	-4.882685	-0.722257	-0.381235	H	7.244126	-3.673639	-1.795831
C	-3.443442	1.144509	-1.158528	H	8.235151	-4.703130	0.227616
C	-1.082556	0.803856	-1.857325	C	3.732050	1.543621	0.539321
C	-4.884491	-4.972487	0.531053	C	3.691202	2.933004	0.270753
C	-6.054386	-2.785785	0.325948	C	6.078349	1.394132	-0.047281
C	-6.078349	-1.394138	0.047293	C	4.839638	3.579494	-0.196986
C	-4.699316	0.667024	-0.688730	C	11.829148	-1.645243	0.506209
C	-3.236204	2.542180	-1.443886	C	7.252905	3.483974	-0.714321
H	-0.231573	0.155955	-2.005281	C	1.743481	4.665514	0.636582
C	-0.954257	2.135583	-2.145968	C	4.699206	-0.667084	0.688685
C	-6.046463	-5.576452	0.930626	C	0.290462	2.438494	1.560748
H	-3.976882	-5.557969	0.471386	C	2.480193	1.090188	1.011811
C	-7.252902	-3.484026	0.714265	C	8.067799	0.259100	0.950533
C	-7.375029	-0.692269	0.172708	C	9.312510	-0.370281	0.867884
C	-5.759031	1.704961	-0.542431	C	4.884517	4.972472	-0.531086
H	-4.041228	3.241285	-1.264560	H	11.288297	-2.387070	1.106786
C	-2.046274	3.019313	-1.923734	H	12.733037	-2.099355	0.098122
H	-0.011341	2.522984	-2.519781	H	12.104677	-0.793146	1.140492
C	-7.252475	-4.821720	1.006837	H	8.182392	2.932352	-0.769615
H	-6.053311	-6.633605	1.180312	C	7.252491	4.821662	-1.006921
H	-8.182403	-2.932429	0.769549	C	0.440509	4.823731	1.101040
C	-8.065343	-0.280068	-0.963792	H	2.273090	5.549647	0.306042
C	-7.954117	-0.454725	1.426076	C	3.443342	-1.144554	1.158212
C	-6.323219	2.282935	-1.685083	C	5.757307	-1.706041	0.538704
C	-6.110981	2.220951	0.708007	H	-0.284726	1.600144	1.920818
H	-1.929641	4.081036	-2.118345	C	-0.283774	3.717584	1.566554
H	-8.177673	-5.312269	1.295058	C	2.306014	-0.256825	1.349471
C	-9.272913	0.398361	-0.856990	H	7.640327	0.439936	1.932331
H	-7.645544	-0.469168	-1.946712	C	2.046076	-3.019436	1.923042
H	-7.433455	-0.782759	2.321678	H	4.040982	-3.241417	1.263714
C	-9.173950	0.198196	1.550662	C	6.986891	-3.284922	-0.813849
H	-6.052500	1.907097	-2.667423	C	7.218346	-3.356995	1.580112
C	-7.213730	3.339425	-1.562882	H	6.063423	-1.897393	2.654523
C	-7.002608	3.287344	0.831768	C	-2.341478	2.919488	2.515160
H	-5.672754	1.783111	1.600408	C	0.954140	-2.135669	2.145549
C	-9.839674	0.640047	0.399823	H	0.231578	-0.155955	2.005264
H	-9.774075	0.727028	-1.760138	H	9.816243	-0.675964	1.776929
H	-9.618566	0.386202	2.522666	H	3.976919	5.557971	-0.471411
C	-7.558179	3.857643	-0.312478	C	6.046491	5.576412	-0.930695
H	-7.642294	3.780004	-2.460128	H	6.053348	6.633559	-1.180403
H	-7.257056	3.667323	1.816960	H	8.177690	5.312192	-1.295175
O	-11.022851	1.295114	0.605371	H	-0.031430	5.800459	1.121534
H	-8.249363	4.691706	-0.235066	C	3.236024	-2.542290	1.443262
C	-11.763517	1.734518	-0.526461	C	6.093958	-2.222483	-0.714841
H	-12.660574	2.210176	-0.127843	C	6.332651	-2.284688	1.675415
H	-12.052752	0.891441	-1.166649	O	-1.546647	3.988179	2.016237
H	-11.197331	2.464374	-1.118110	C	1.082503	-0.803898	1.857138