

Electronic Supplementary Information

Effects of the Acceptor Unit in Dyes with Acceptor-Bridge-Donor Architecture in the Electron Photo-Injection Mechanism and Aggregation in DSSCs

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KEYWORDS: Solar cell, injection mechanism, organic dyes, DFT.

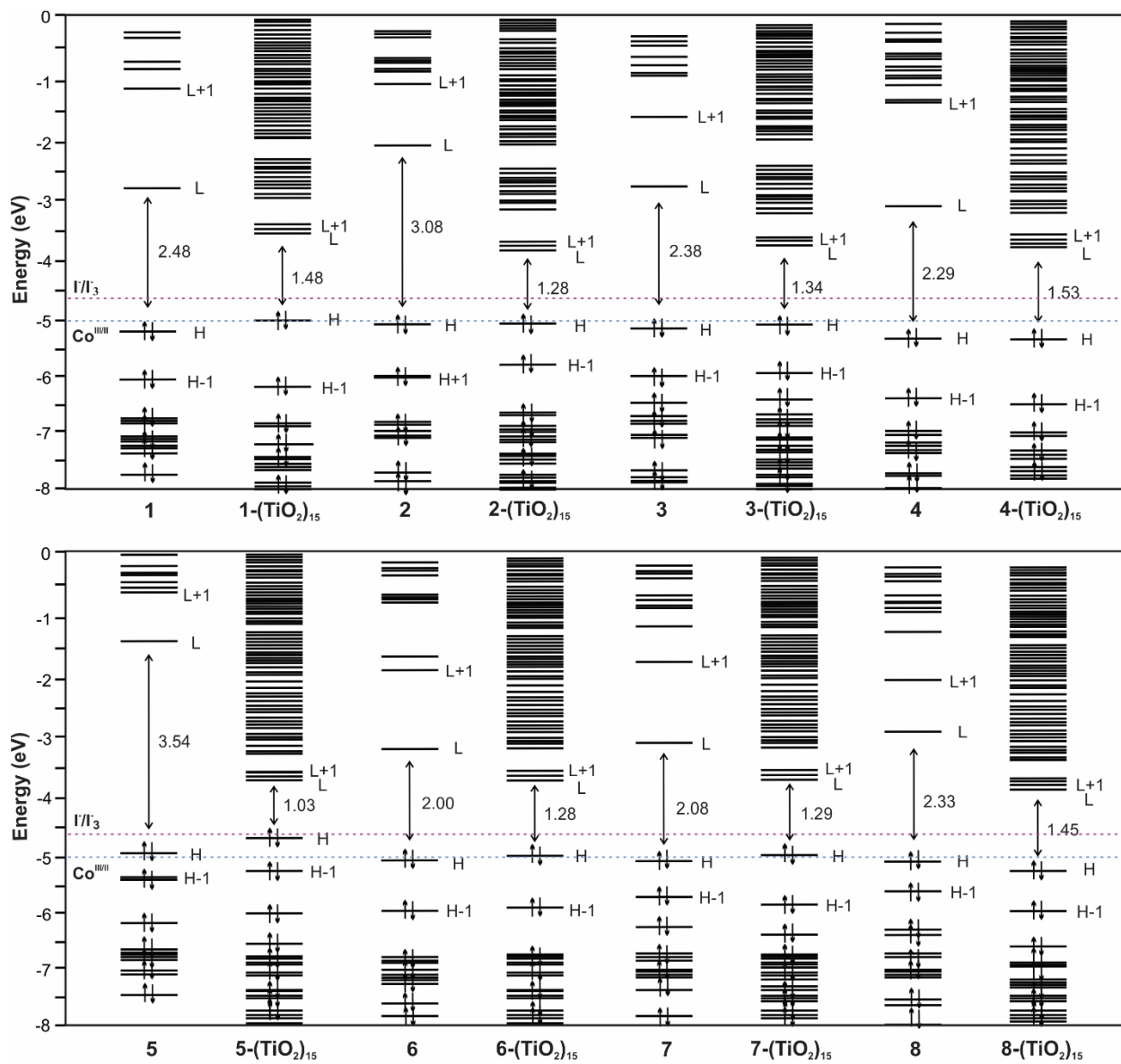


Figure S1 Energy levels diagram of the free dyes and dyes adsorbed to the TiO₂ cluster (Dye-(TiO₂)₁₅) using the B3LYP functional.

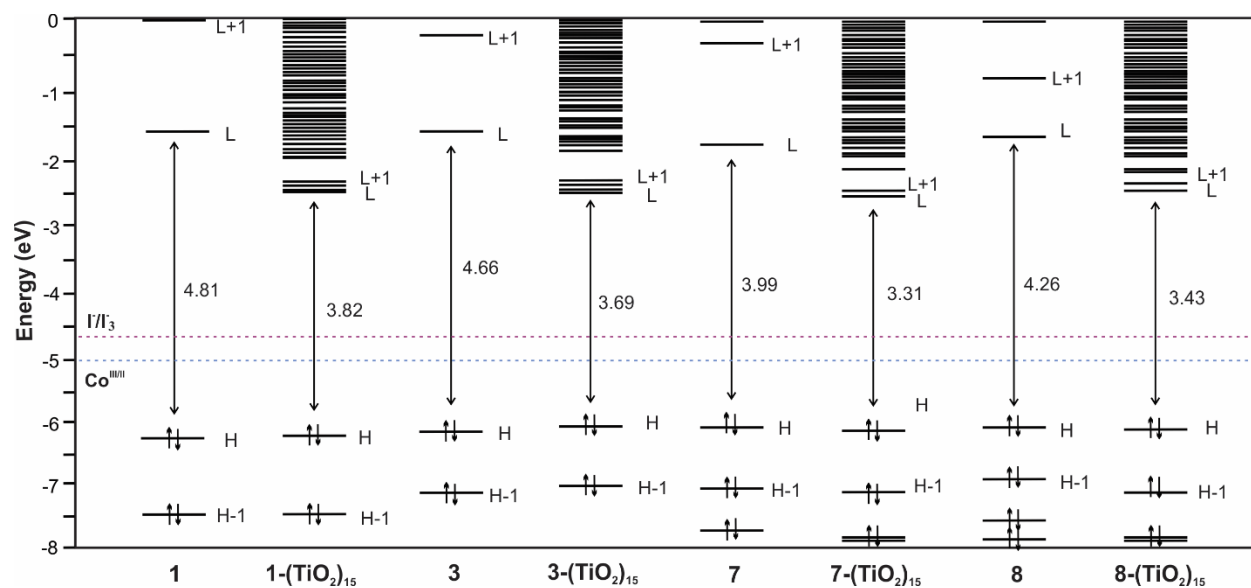


Figure S2 Energy levels diagram of the free dyes and dyes adsorbed to the TiO_2 cluster (Dye- $(\text{TiO}_2)_{15}$) using the CAM-B3LYP functional.

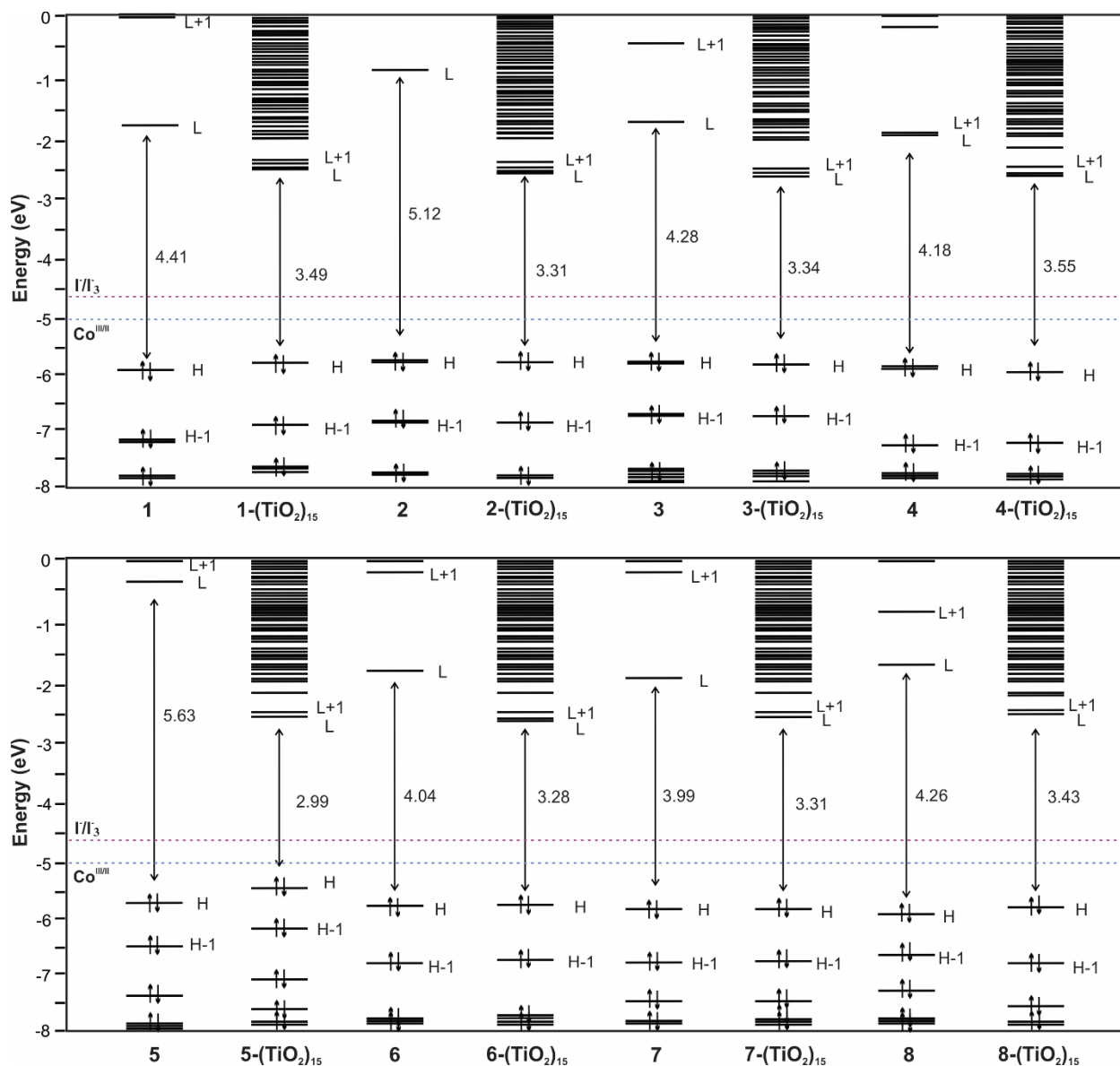


Figure S3 Energy levels diagram of the free dyes and dyes adsorbed to the TiO_2 cluster (Dye- $(\text{TiO}_2)_{15}$) using the BHandHLYP functional.

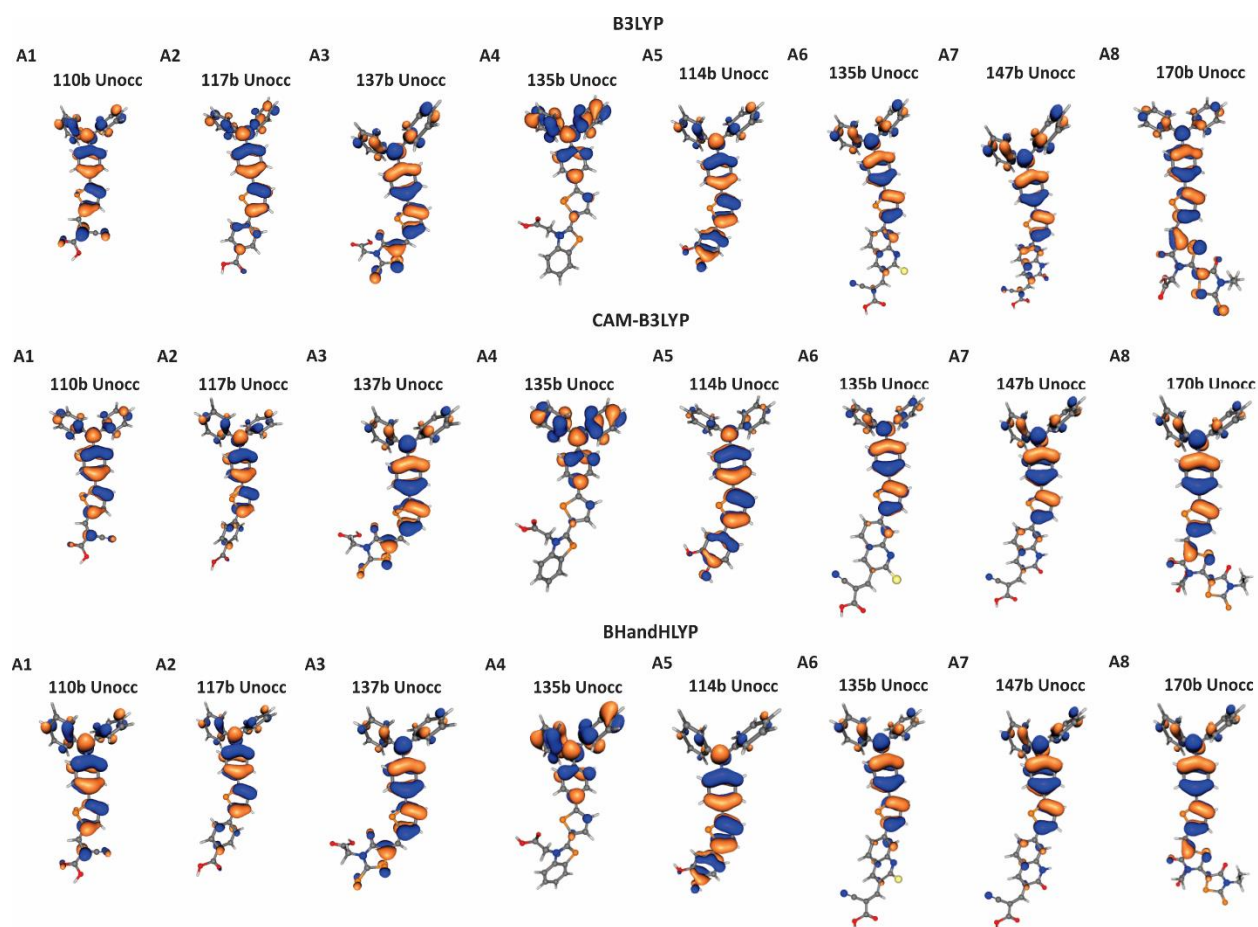


Figure S4. Molecular orbitals isosurfaces of the hole generated by the oxidation process of all the dyes.

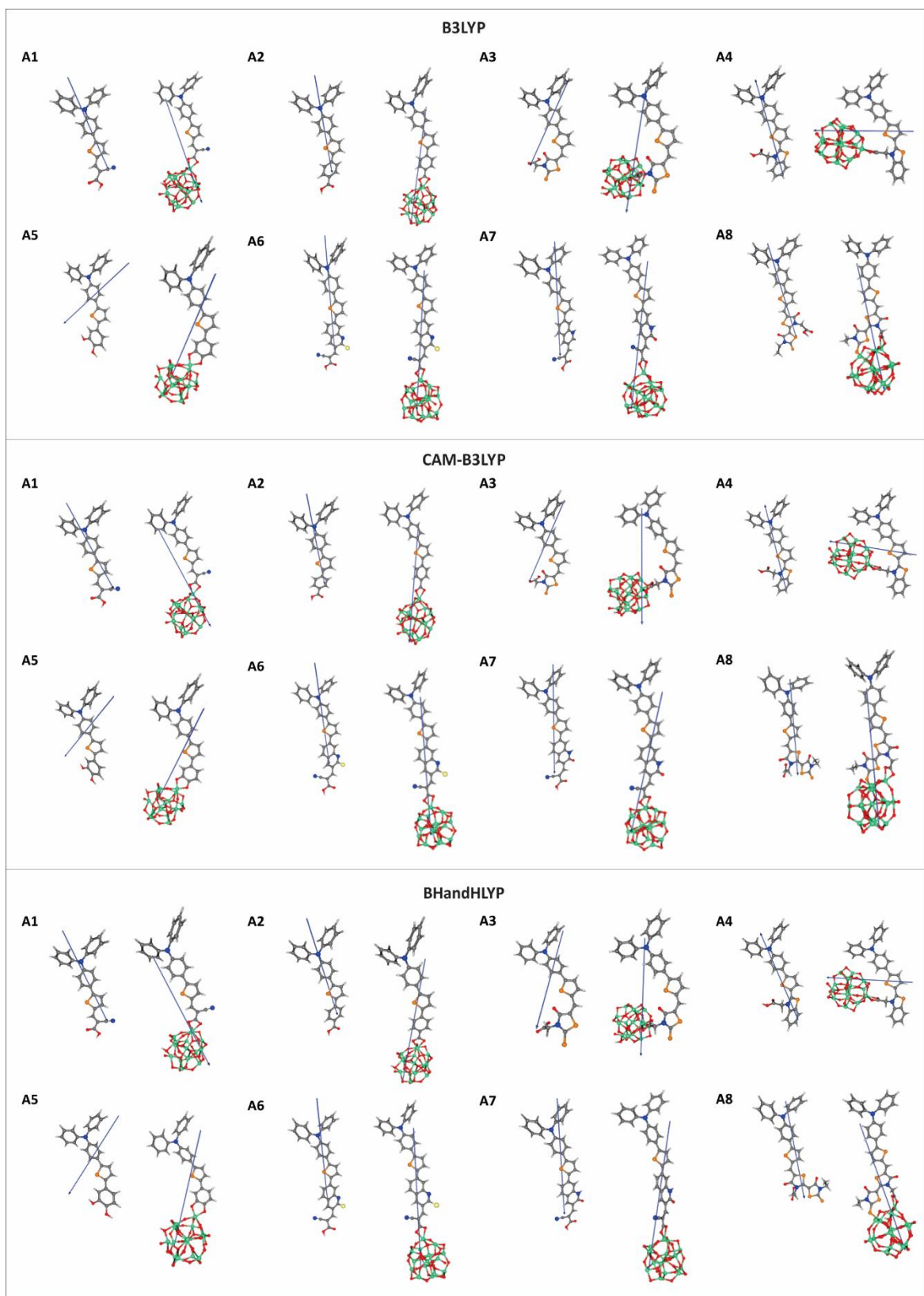


Figure S5 Dipole moment vectors of the free dyes and the dye-(TiO₂)₁₅ systems.

Table S1. Calculated (Calc., [eV]) and experimental (Exp., [nm]) maximum absorption wavelengths, active molecular orbitals (MO) and their contributions in %. Maximum absorption wavelengths for UV–Vis absorption spectra of all dyes computed using TD-B3LYP. Left panel: free dyes and right panel: dye-(TiO₂)₁₅.

Dyes	Exp.*	Calc.	<i>f</i>	Active MO		Contr. %	Exp.*	Calc.	<i>f</i>	Active MO		Contr. %
A1	404(3.07)	561(2.21)	0.848	HOMO	→	LUMO	99	404(3.07)	608(2.04)	0.305	HOMO → LUMO+2 HOMO → LUMO+3	9.7 87
A2		455(2.72)	0.910	HOMO	→	LUMO	99		492(2.52)	0.853	HOMO → LUMO+8 HOMO → LUMO+9	39 51
A3		589(2.11)	0.865	HOMO	→	LUMO	99		596(2.08)	0.950	HOMO → LUMO+6	100
A4		598(2.07)	1.271	HOMO	→	LUMO	100		604(2.05)	0.506	HOMO → LUMO+3 HOMO → LUMO+4	38 57
A5		400(3.10)	1.155	HOMO	→	LUMO	99		784(1.58)	0.116	HOMO → LUMO+4 HOMO → LUMO+5	10 78
A6		694(1.79)	0.675	HOMO	→	LUMO	99		749(1.66)	0.677	HOMO → LUMO+2 HOMO → LUMO+3	96 4
A7		669(1.85)	0.682	HOMO	→	LUMO	99		738(1.68)	0.763	HOMO → LUMO+2 HOMO → LUMO+3	89 9
A8		606(2.05)	1.367	HOMO	→	LUMO	100		716(1.73)	0.611	HOMO → LUMO+3	97

*Ref: Hagberg, D. P.; Marinado, T.; Karlsson, K. M.; Nonomura, K.; Qin, P.; Boschloo, G.; Brinck, T.; Hagfeldt, A.; Sun, L.; Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. J. Org. Chem. 2007, 72, 9550-9556.

Table S2. Calculated (Calc., [eV]) and experimental (Exp., [nm]) maximum absorption wavelengths, active molecular orbitals (MO) and their contributions in %. Maximum absorption wavelengths for UV–Vis absorption spectra of all dyes computed using TD-CAM-B3LYP. Left panel: free dyes and right panel: dye-(TiO₂)₁₅.

Dyes	Exp.*	Calc.	<i>f</i>	Active MO			Contr. %	Exp.*	Calc.	<i>f</i>	Active MO			Contr. %
A1	404(3.07)	415(2.99)	1.360	HOMO	→	LUMO	80	404(3.07)	471(2.63)	1.851	HOMO	→	LUMO+2	50
				HOMO-1	→	LUMO	14				HOMO	→	LUMO+3	19
A2		349(3.55)	1.498	HOMO	→	LUMO	70		381(3.25)	1.400	HOMO-1	→	LUMO+5	8
				HOMO-1	→	LUMO	15				HOMO	→	LUMO+1	20
				HOMO	→	LUMO+1	13				HOMO	→	LUMO+5	37
A3		438(2.83)	1.390	HOMO	→	LUMO	72		467(2.66)	1.437	HOMO-1	→	LUMO+2	15
				HOMO-1	→	LUMO	10				HOMO	→	LUMO+2	78
A4		439(2.83)	1.320	HOMO	→	LUMO	79		473(2.62)	1.238	HOMO-1	→	LUMO+2	12
				HOMO-1	→	LUMO	14				HOMO	→	LUMO+2	82
A5		332(3.73)	1.410	HOMO	→	LUMO	85		426(2.91)	0.209	HOMO-1	→	LUMO+4	9
				HOMO-1	→	LUMO+3	5				HOMO	→	LUMO+2	6
											HOMO	→	LUMO+3	13
											HOMO	→	LUMO+4	20
A6		400(3.10)	1.630	HOMO	→	LUMO	56		450(2.76)	2.031	HOMO-1	→	LUMO+2	20
				HOMO-1	→	LUMO	24				HOMO	→	LUMO+2	58
				HOMO		LUMO+1	5							
A7		425(2.92)	1.737	HOMO	→	LUMO	46		469(2.64)	2.211	HOMO-1	→	LUMO+2	30
				HOMO-1	→	LUMO	39				HOMO	→	LUMO+2	50
A8		436(2.84)	1.934	HOMO	→	LUMO	61		486(2.55)	1.964	HOMO-1	→	LUMO+2	18
				HOMO-1	→	LUMO	27				HOMO	→	LUMO+2	47

*Ref: Hagberg, D. P.; Marinado, T.; Karlsson, K. M.; Nonomura, K.; Qin, P.; Boschloo, G.; Brinck, T.; Hagfeldt, A.; Sun, L.; Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. J. Org. Chem. 2007, 72, 9550-9556.

Table S3. Calculated (Calc., [eV]) and experimental (Exp., [nm]) maximum absorption wavelengths, active molecular orbitals (MO) and their contributions in %. Maximum absorption wavelengths for UV–Vis absorption spectra of all dyes computed using TD-BHandHLYP. Left panel: free dyes and right panel: dye-(TiO₂)₁₅.

Dyes	Exp.*	Calc.	<i>f</i>	Active MO			Contr. %	Exp.	Calc.	<i>f</i>	Active MO			Contr. %
A1	404(3.07)	415(2.99)	1.366	HOMO	→	LUMO	85	404(3.07)	468(2.65)	1.814	HOMO-1	→	LUMO+2	7
				HOMO-1	→	LUMO	10				HOMO	→	LUMO+2	76
							HOMO				→	LUMO+3	5	
A2		348(3.56)	1.488	HOMO	→	LUMO	77		387(3.21)	1.745	HOMO-1	→	LUMO+8	54
				HOMO-1	→	LUMO	12				HOMO	→	LUMO+3	7
				HOMO	→	LUMO+1	9				HOMO	→	LUMO+8	32
A3		433(2.86)	1.424	HOMO	→	LUMO	79		463(2.68)	1.460	HOMO-1	→	LUMO+3	11
				HOMO-1	→	LUMO	12				HOMO	→	LUMO+3	83
A4		440(2.82)	1.350	HOMO	→	LUMO	86		471(2.63)	1.272	HOMO-1	→	LUMO+2	8
				HOMO-1	→	LUMO	9.5				HOMO	→	LUMO+2	87
A5		328(3.78)	1.420	HOMO	→	LUMO	87		436(2.85)	0.145	HOMO-1	→	LUMO+5	5
				HOMO-1	→	LUMO	3				HOMO	→	LUMO+2	9
							HOMO				→	LUMO+3	15	
							HOMO				→	LUMO+4	12	
							HOMO				→	LUMO+5	24	
A6		411(3.01)	1.491	HOMO	→	LUMO	71		466(2.66)	1.833	HOMO-1	→	LUMO+2	14
				HOMO-1	→	LUMO	17				HOMO	→	LUMO+2	72
A7		431(2.88)	1.716	HOMO	→	LUMO	64		478(2.60)	2.076	HOMO-1	→	LUMO+2	20
				HOMO-1	→	LUMO	26				HOMO	→	LUMO+2	67
A8		430(2.88)	1.927	HOMO	→	LUMO	72		483(2.57)	1.896	HOMO-1	→	LUMO+2	12
				HOMO-1	→	LUMO	18				HOMO	→	LUMO+2	54

*Ref: Hagberg, D. P.; Marinado, T.; Karlsson, K. M.; Nonomura, K.; Qin, P.; Boschloo, G.; Brinck, T.; Hagfeldt, A.; Sun, L.; Tuning the HOMO and LUMO Energy Levels of Organic Chromophores for Dye Sensitized Solar Cells. J. Org. Chem. 2007, 72, 9550-9556.

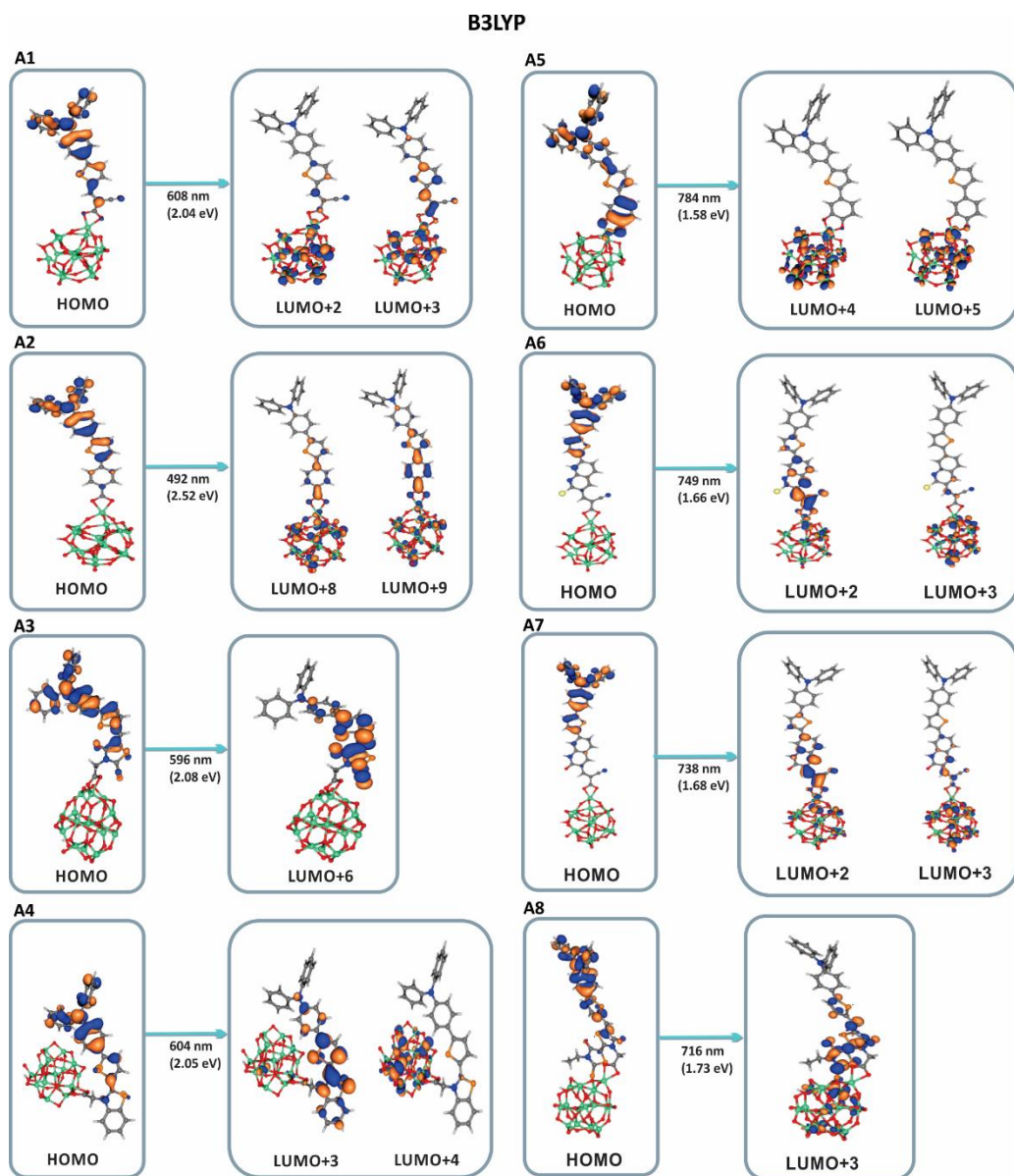


Figure S6 Active molecular orbitals isosurfaces of the computed vertical transitions of Dye-(TiO₂)₁₅ systems using the TD-B3LYP functional.

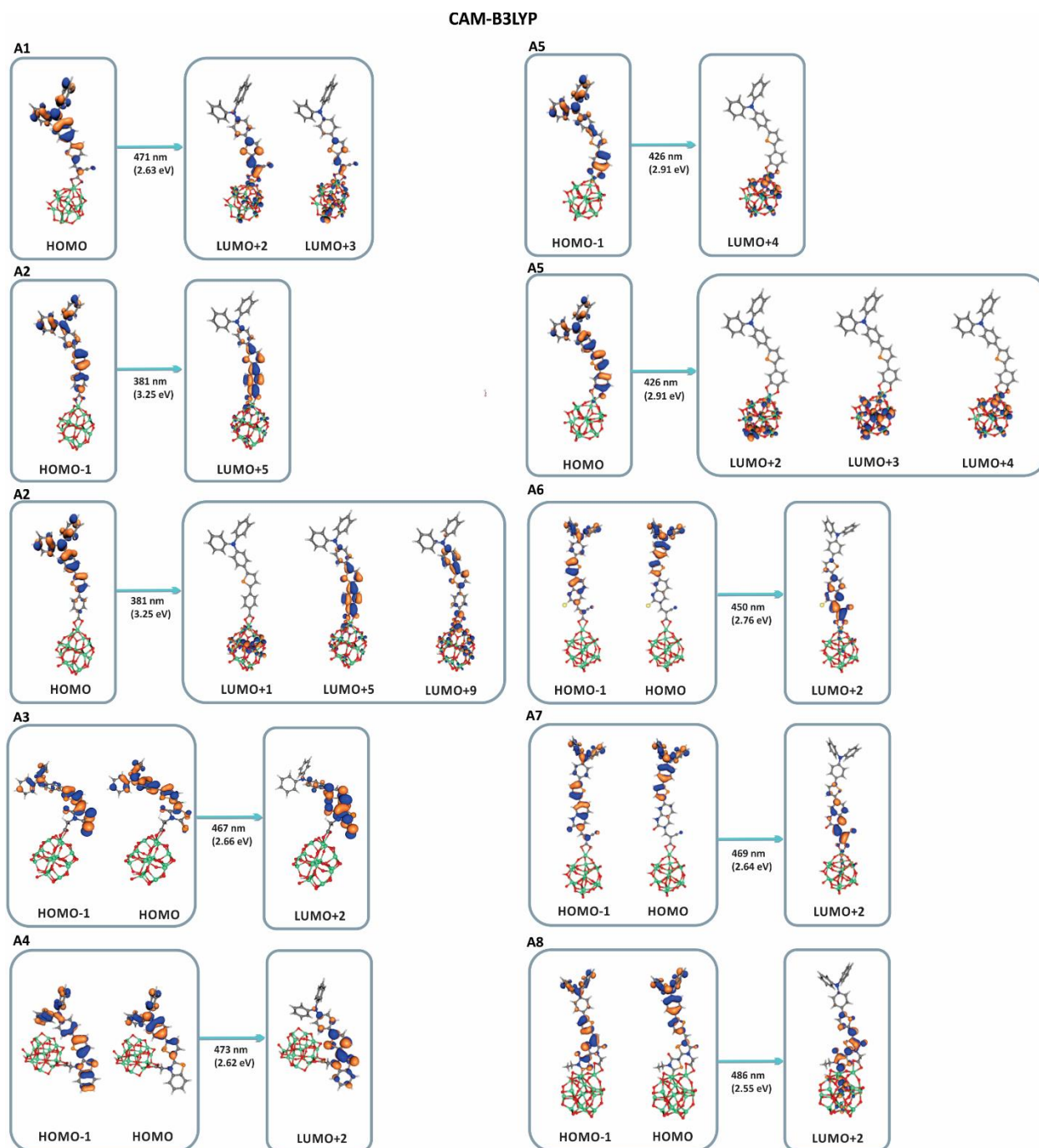


Figure S7 Active molecular orbitals isosurfaces of the computed vertical transitions of Dye-(TiO₂)₁₅ systems using the TD-CAM-B3LYP functional.

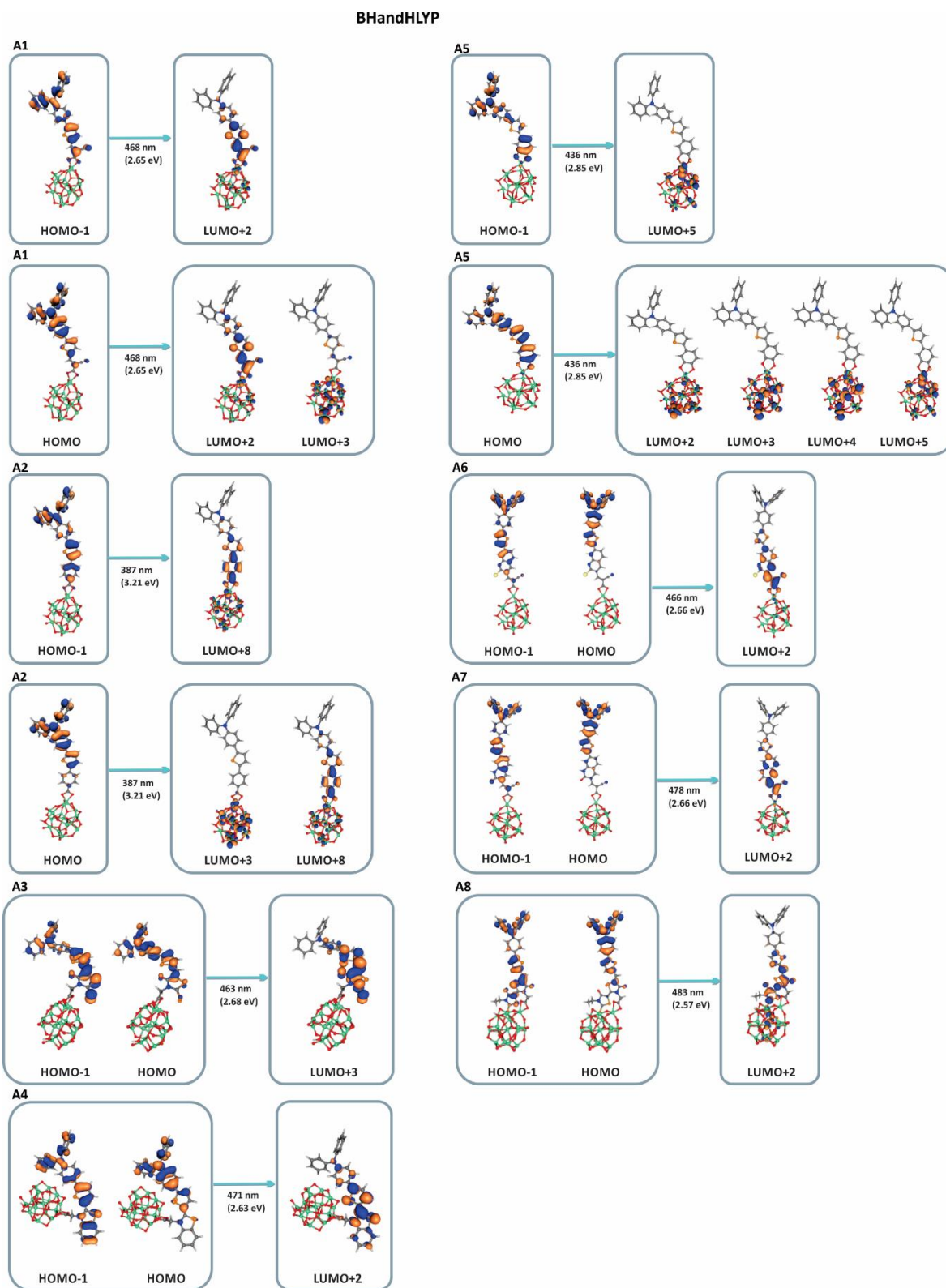


Figure S8 Active molecular orbitals isosurfaces of the computed vertical transitions of Dye-(TiO₂)₁₅ systems using the TD-BHandHLYP functional.

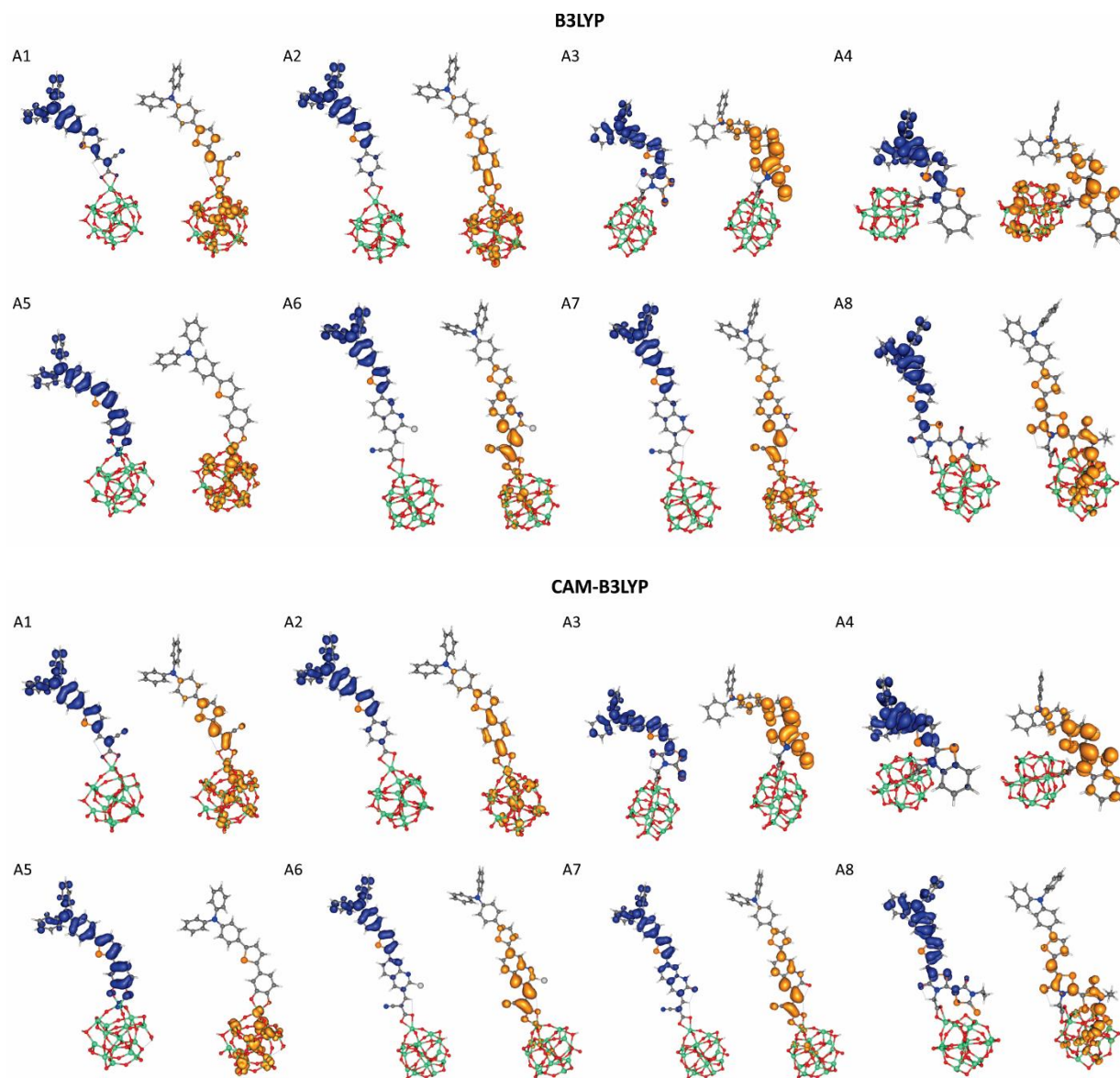


Figure S9 EDDMs for the **A-bridge-D-(TiO₂)₁₅** systems upon photoexcitation to the first singlet excitation. The blue densities represent the source of electrons and the orange densities represent the target location after electron transfer.

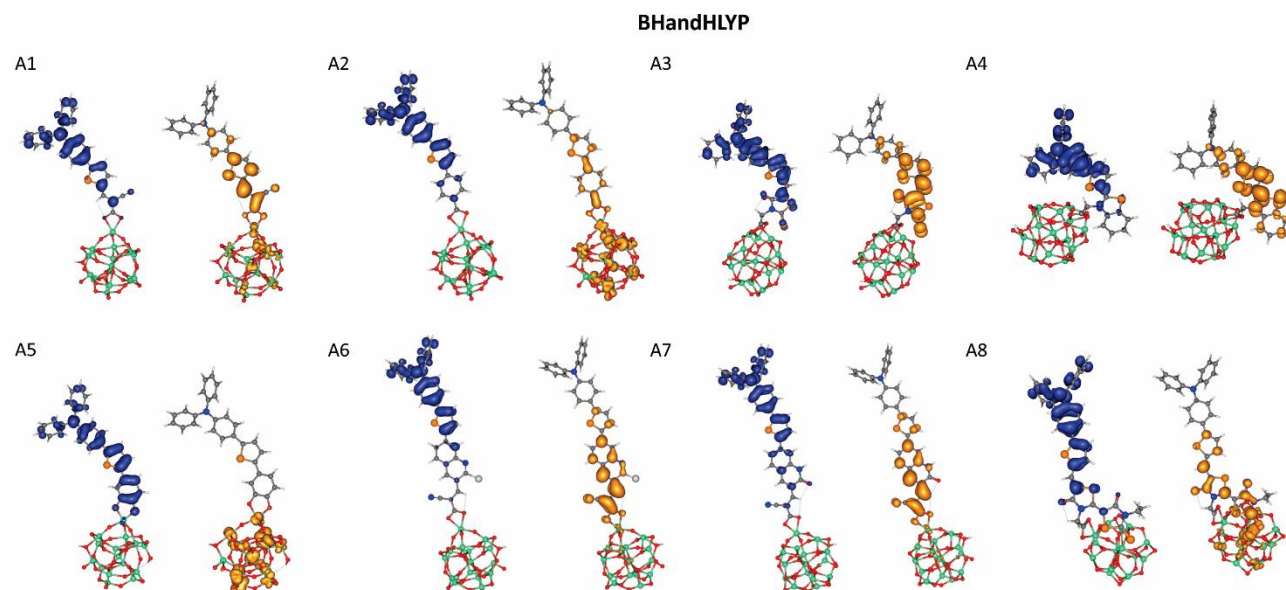


Figure S10 EDDMs for the **A-bridge-D-(TiO₂)₁₅** systems upon photoexcitation to the first singlet excitation. The blue densities represent the source of electrons and the orange densities represent the target location after electron transfer.

Table S4. Calculated negative free energy of the injection ($-\Delta G^{\text{inj}}$), driving force for charge recombination (ΔG^0_{rec}), light-harvesting efficiency (LHE) for the lowest singlet excited state, the open-circuit voltage (eV_{OC}), dipole moments (μ) and HOMO-LUMO gap (H-L) for the selected family of A-bridge-D dyes.

	A	$-\Delta G^{\text{inj}}$	ΔG^0_{rec}	LHE	eV_{OC}	μ dye	μ dye-TiO ₂	H-L GAP dye	H-L GAP dye-TiO ₂
B3LYP	A1	1.03	1.18	0.86	1.29	9.25	15.28	2.48	1.48
	A2	1.69	1.03	0.88	2.05	4.70	8.84	3.08	1.28
	A3	1.00	1.11	0.86	1.27	11.50	15.14	2.38	1.34
	A4	0.69	1.38	0.95	0.91	12.51	29.49	2.29	1.53
	A5	2.17	0.93	0.93	-	1.98	17.14	3.54	1.03
	A6	0.74	1.05	0.79	0.95	8.62	17.14	2.00	1.28
	A7	0.79	1.06	0.79	1.02	11.97	15.49	2.08	1.29
	A8	-0.97	1.08	0.96	1.25	12.65	10.42	2.33	1.45
CAM-B3LYP	A1	0.61	2.38	0.96	2.43	7.46	13.34	4.81	3.82
	A2	1.28	2.27	0.97	3.27	3.90	7.81	5.54	3.67
	A3	0.51	2.32	0.96	2.34	10.77	14.01	4.66	3.69
	A4	0.31	2.52	0.97	2.05	17.52	30.31	4.57	3.89
	A5	1.54	2.19	0.96	-	2.17	18.10	6.03	3.41
	A6	0.82	2.28	0.98	2.19	5.88	7.83	4.47	3.64
	A7	0.64	2.28	0.98	2.14	9.76	13.29	4.42	3.66
	A8	0.53	2.31	0.99	2.32	10.86	20.58	4.63	3.79
BHandHLYP	A1	0.90	2.09	0.96	2.32	8.17	14.25	4.41	3.49
	A2	1.60	1.96	0.97	3.17	4.22	8.25	5.12	3.31
	A3	0.84	2.02	0.96	2.26	11.30	14.62	4.28	3.34
	A4	0.58	2.24	0.96	1.94	17.52	30.46	4.18	3.55
	A5	1.91	1.87	0.96	-	2.48	19.21	5.63	2.99
	A6	1.04	1.97	0.97	2.07	5.88	8.61	4.04	3.28
	A7	0.91	1.97	0.98	2.02	10.65	14.29	3.99	3.31
	A8	0.88	2.00	0.99	2.26	11.34	20.96	4.26	3.43

A2

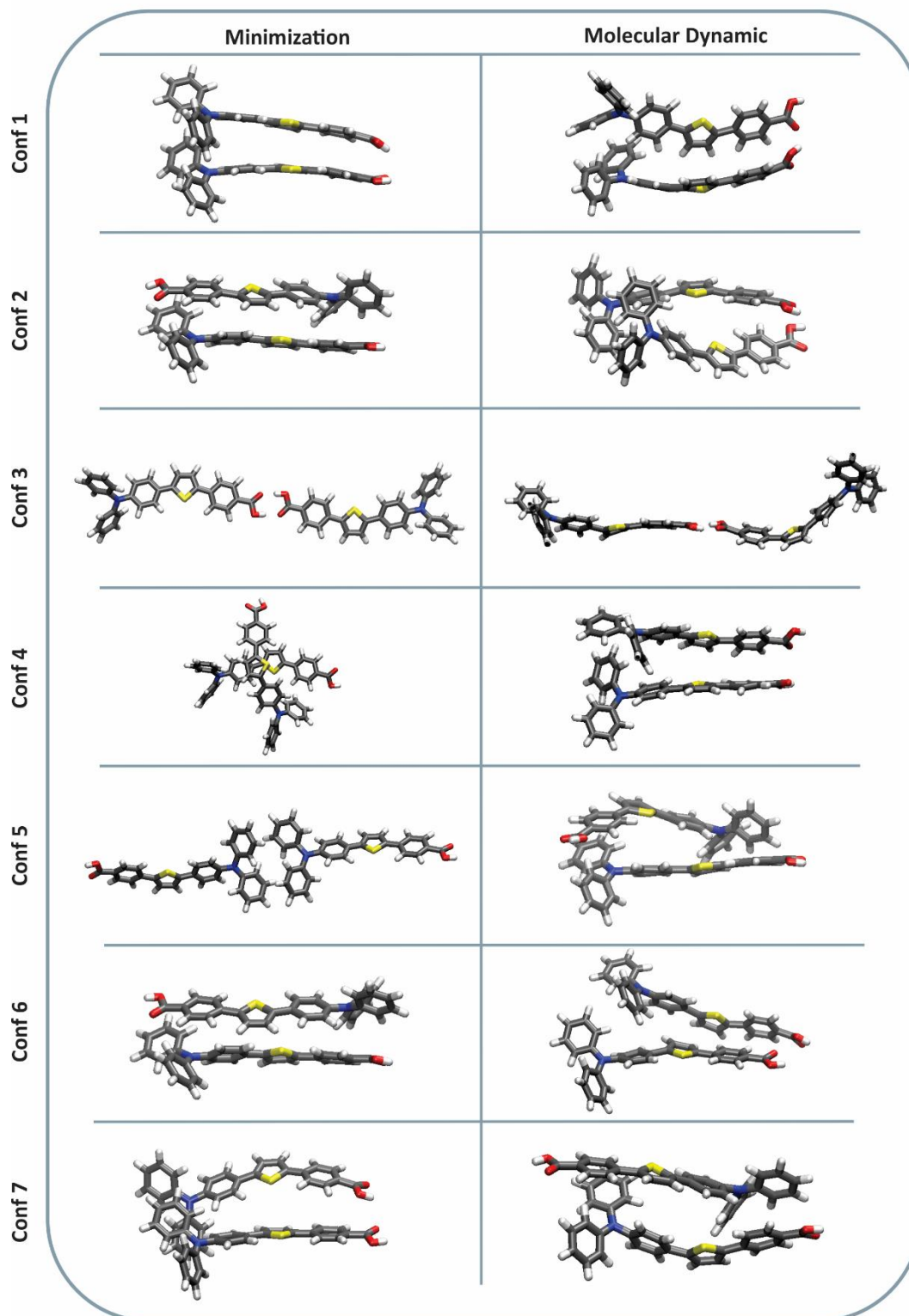


Figure S11 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for **A2**.

A3

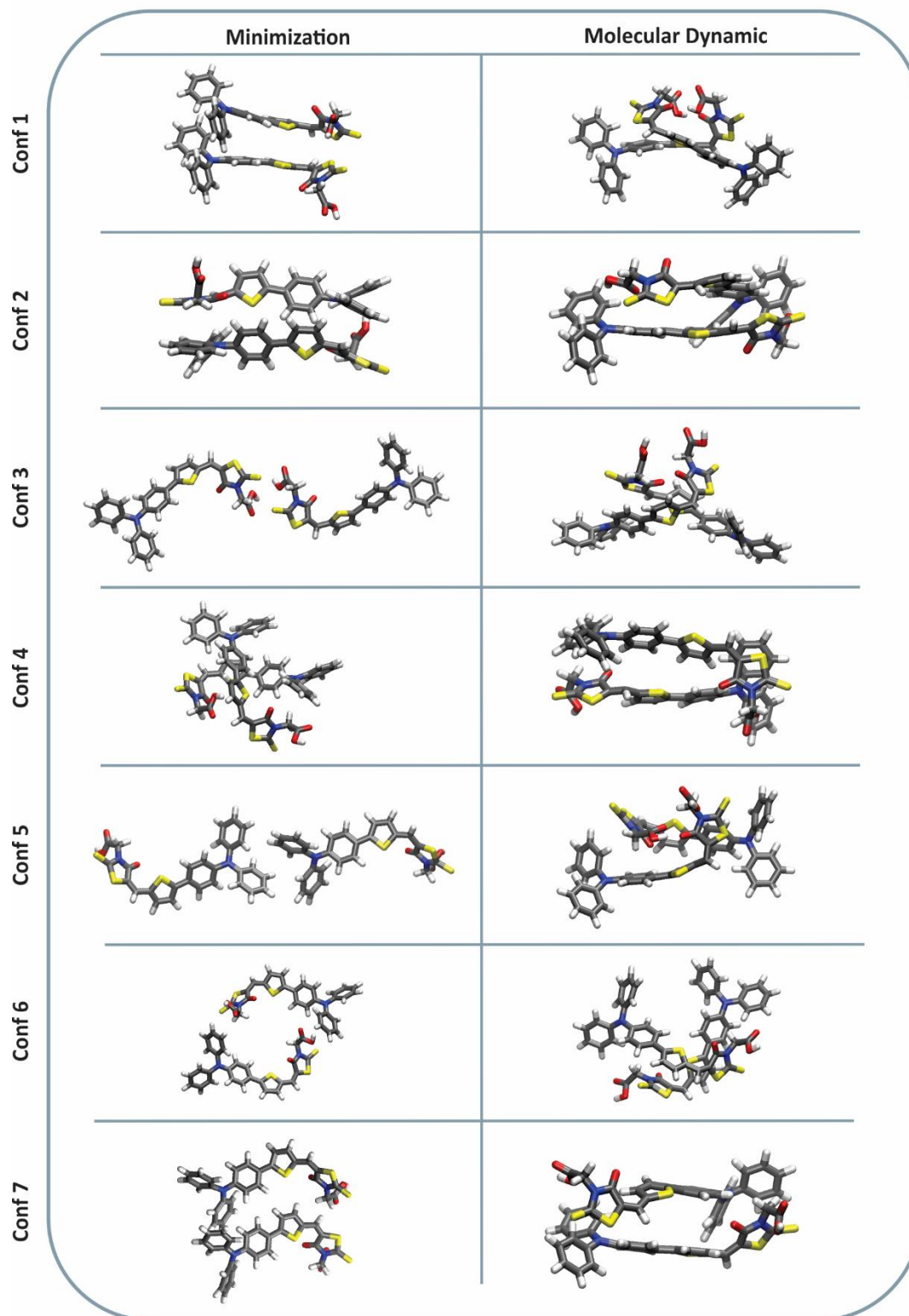


Figure S12 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for A3.

A4

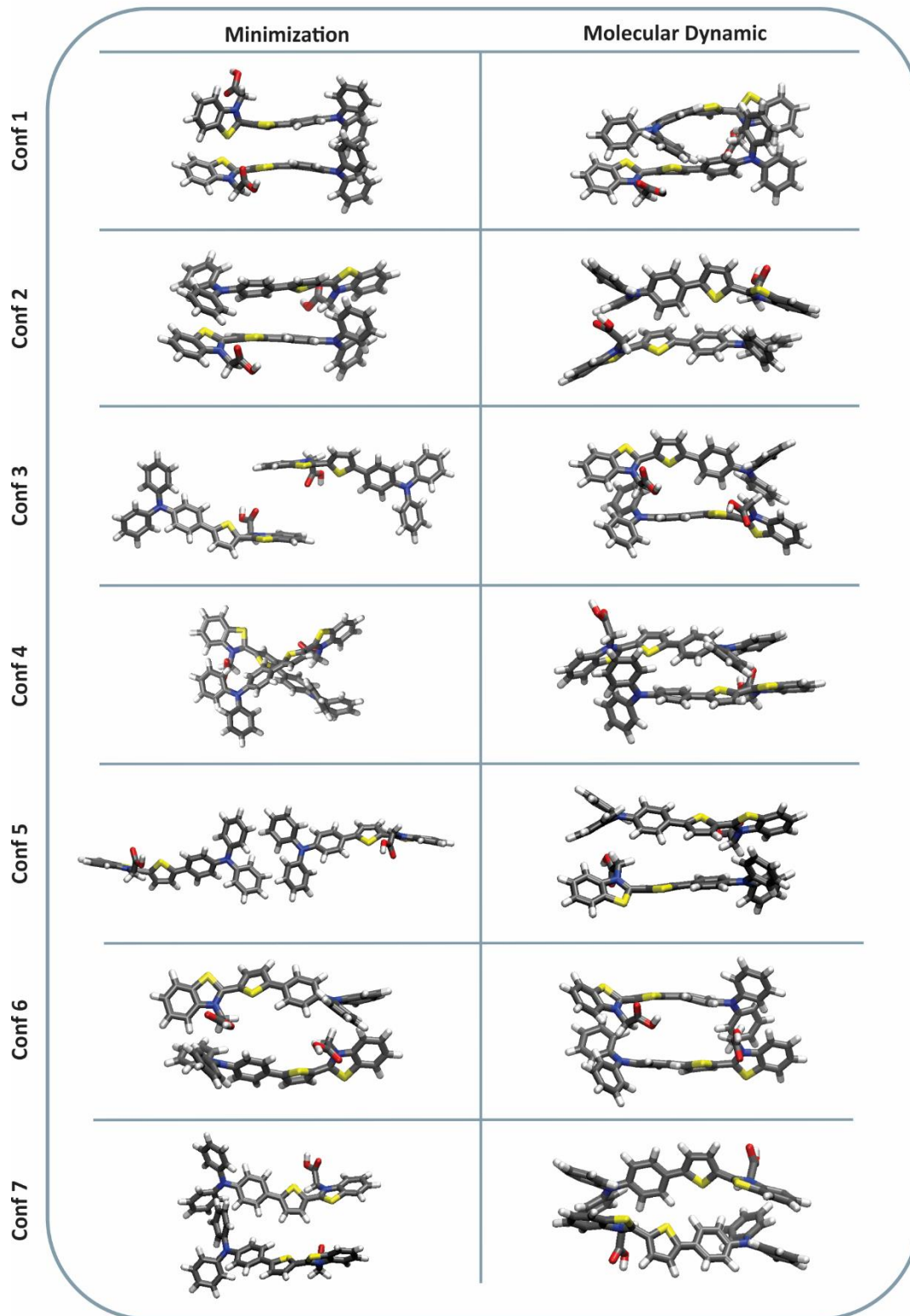


Figure S13 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for **A4**.

A5

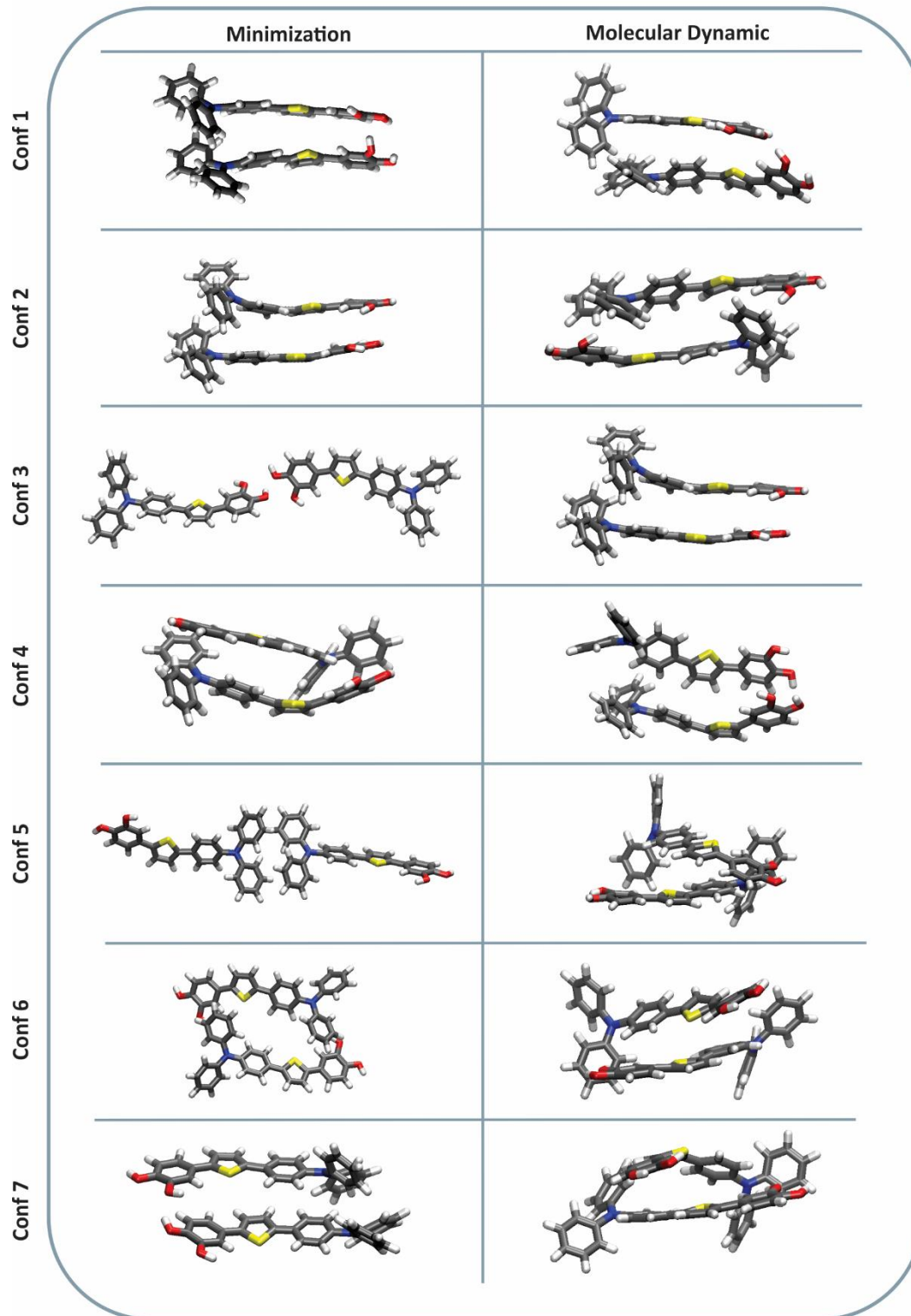


Figure S14 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for A5.

A6

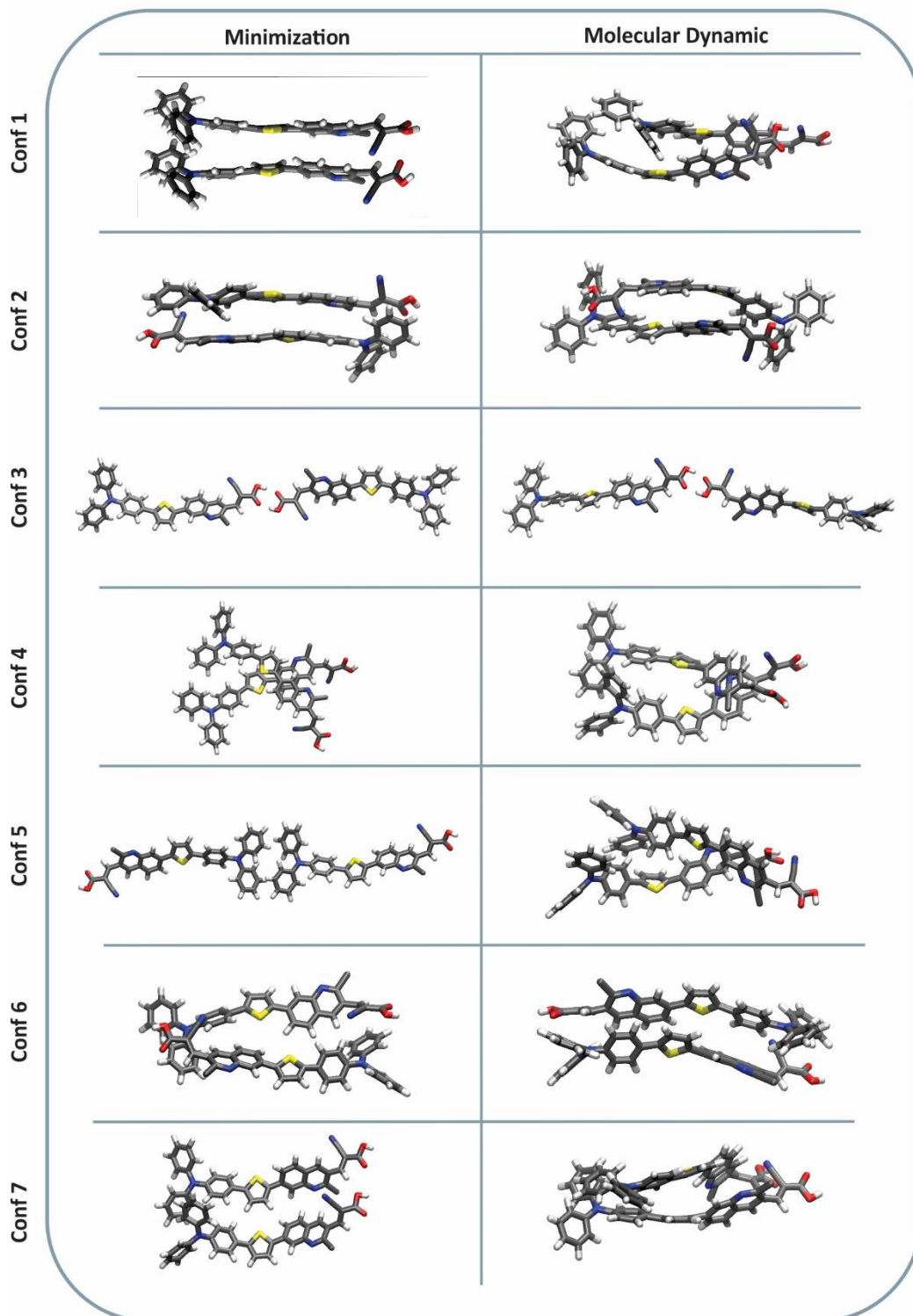


Figure S15 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for **A6**.

A7

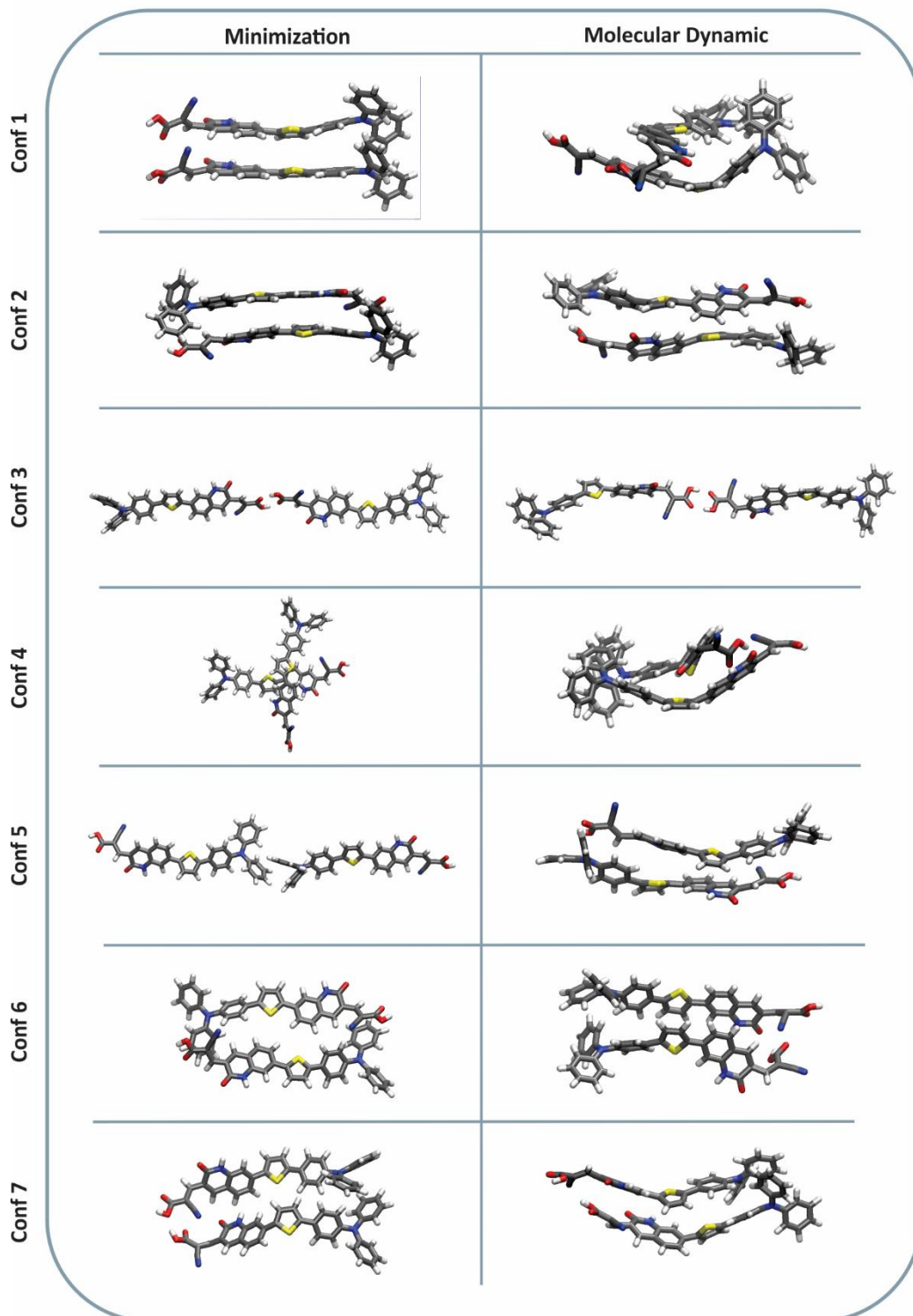


Figure S16 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for A7.

A8

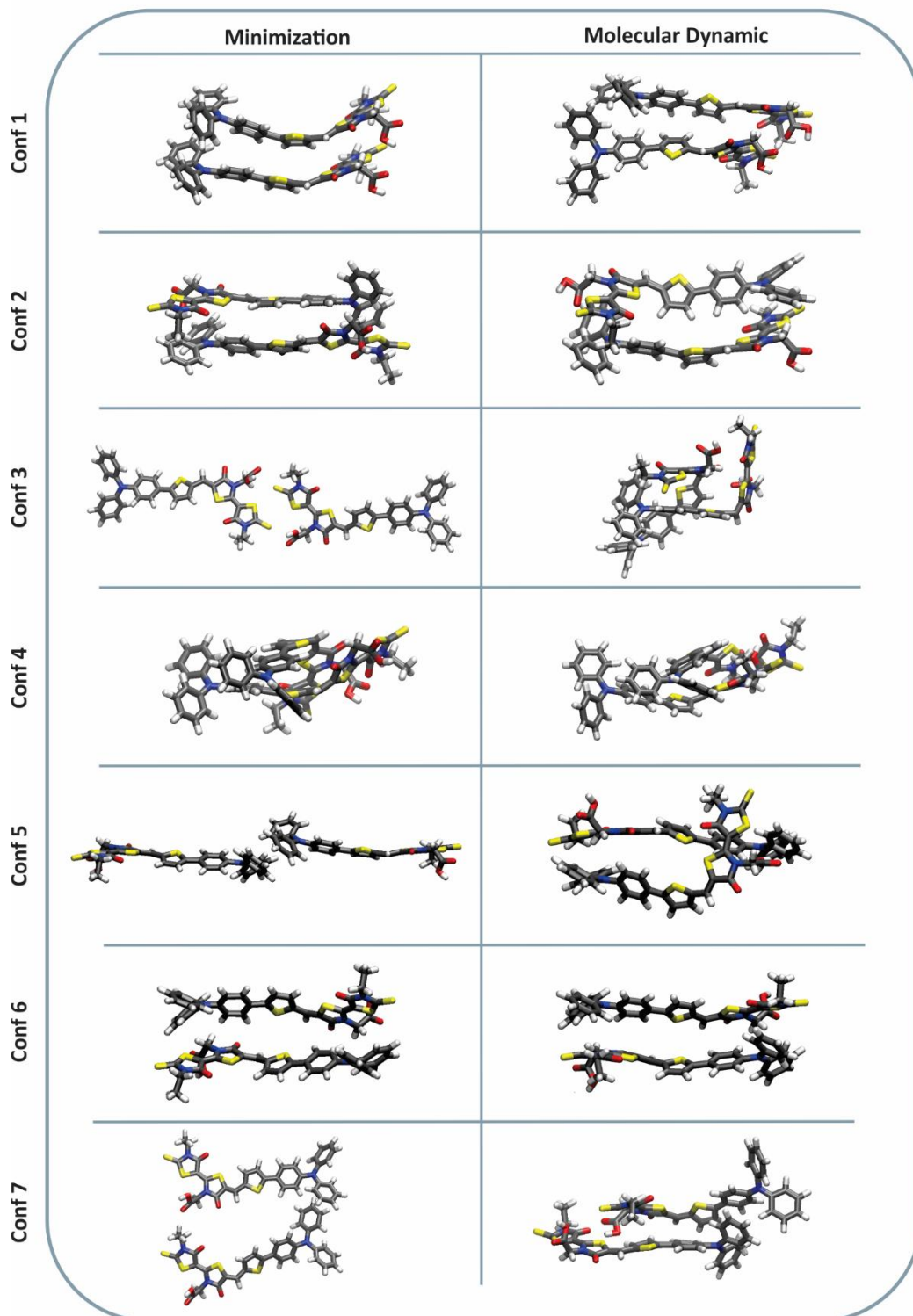


Figure S17 Obtained structures of the minimized systems and of the molecular dynamics starting from the proposed configurations for **A8**.

Table S5. Dimer interaction energies (ΔE) calculated from MD and minimized geometries.

		Minimization				Dynamics			$ \Delta E_{nb} $ (kcal mol ⁻¹)
		Monomer E (kcal mol ⁻¹)	Dimer E (kcal mol ⁻¹)	ΔE (kcal mol ⁻¹)		Monomer E (kcal mol ⁻¹)	Dimer E (kcal mol ⁻¹)	ΔE (kcal mol ⁻¹)	
A1	Conf 1		9.72	-19.11			95.31	-20.86	1.76
	Conf 2		6.14	-22.69			95.57	-20.61	2.08
	Conf 3		13.74	-15.08			101.90	-14.28	0.80
	Conf 4	14.41	8.16	-20.66	58.09		96.09	-20.09	0.58
	Conf 5		22.70	-6.13			104.94	-11.23	5.11
	Conf 6		12.07	-16.76			99.64	-16.54	0.21
	Conf 7		15.21	-13.62			99.09	-17.09	3.47
A2	Conf 1		127.94	-19.73			225.47	-17.98	1.75
	Conf 2		128.61	-19.06			227.42	-16.03	3.02
	Conf 3		129.89	-17.77			227.16	-16.29	1.49
	Conf 4	73.83	133.05	-14.61	121.72		230.60	-12.85	1.76
	Conf 5		141.36	-6.31			233.75	-9.70	3.38
	Conf 6		128.81	-18.85			230.45	-13.00	5.85
	Conf 7		131.31	-16.36			228.74	-14.71	1.65
A3	Conf 1		34.07	-18.30			125.43	-27.16	8.86
	Conf 2		23.41	-28.95			127.23	-25.36	3.60
	Conf 3		45.29	-7.07			137.66	-14.93	7.85
	Conf 4	26.18	30.71	-21.65	76.29		129.90	-22.68	1.03
	Conf 5		48.14	-4.22			136.75	-15.84	11.62
	Conf 6		43.00	-9.36			134.28	-18.31	8.95
	Conf 7		40.15	-12.22			133.64	-18.95	6.74
A4	Conf 1		158.20	-14.22			258.68	-21.07	6.85
	Conf 2		141.53	-30.88			248.33	-31.42	0.53
	Conf 3		168.99	-3.43			261.05	-18.70	15.28
	Conf 4	86.21	149.84	-22.57	139.87		255.05	-24.70	2.13
	Conf 5		166.61	-5.80			263.92	-15.83	10.03
	Conf 6		142.32	-30.09			253.29	-26.46	3.63
	Conf 7		167.41	-5.01			263.30	-16.45	11.44
A5	Conf 1		127.73	-30.48			219.14	-25.64	4.84
	Conf 2		140.32	-17.89			226.14	-18.64	0.75
	Conf 3		145.46	-12.76			229.56	-15.22	2.46
	Conf 4	79.11	137.27	-20.94	122.39		226.82	-17.96	2.98
	Conf 5		151.71	-6.51			234.11	-10.67	4.17
	Conf 6		144.91	-13.30			230.23	-14.55	1.26
	Conf 7		137.52	-20.69			225.83	-18.95	1.74
A6	Conf 1		105.30	-27.43			218.91	-28.90	1.47
	Conf 2		97.71	-35.02			214.37	-33.44	1.58
	Conf 3		117.11	-15.61			231.38	-16.43	0.82
	Conf 4	66.36	112.19	-20.53	123.91		226.91	-20.90	0.37
	Conf 5		126.74	-5.99			232.08	-15.73	9.74
	Conf 6		111.12	-21.61			225.19	-22.62	1.02
	Conf 7		110.27	-22.46			222.77	-25.04	2.59
A7	Conf 1		40.26	-26.73			154.80	-29.13	2.40
	Conf 2		34.83	-32.16			153.77	-30.16	2.01
	Conf 3		50.79	-16.20			167.33	-16.60	0.39
	Conf 4	33.50	50.50	-16.50	91.96		160.39	-23.53	7.03
	Conf 5		62.08	-4.92			167.24	-16.69	11.77
	Conf 6		48.39	-18.61			161.90	-22.02	3.42
	Conf 7		45.43	-21.56			157.16	-26.76	5.20
A8	Conf 1		9.73	-32.98			133.68	-32.43	0.55
	Conf 2		4.12	-38.59			128.92	-37.20	1.39
	Conf 3		31.12	-11.59			145.14	-20.97	9.37
	Conf 4	21.36	15.27	-27.45	83.06		139.58	-26.54	0.91
	Conf 5		31.11	-11.61			146.16	-19.96	8.35
	Conf 6		31.09	-11.62			145.88	-20.23	8.61
	Conf 7		35.52	-7.19			146.46	-19.66	12.47

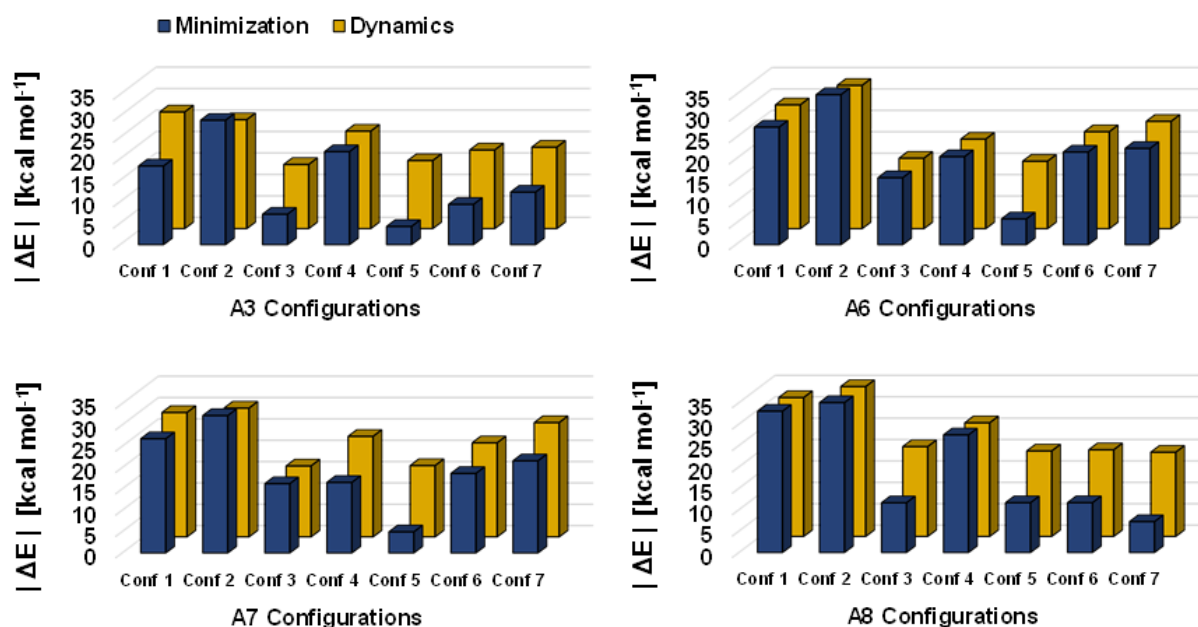
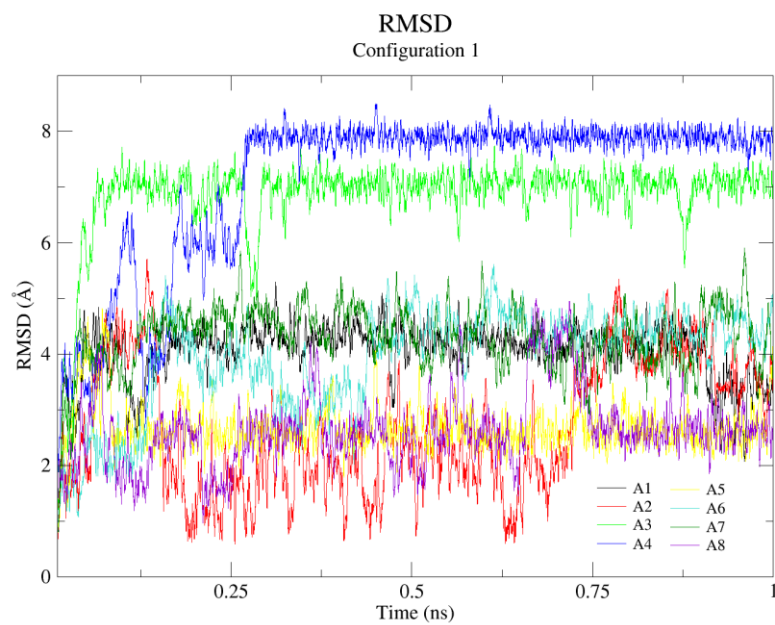


Figure S18 Dimer interaction energies (ΔE) for A3, A6, A7 and A8 dyes calculated using eq. 5. Yellow bars refer to interaction energies calculated from MD structures while blue bars correspond to the minimized geometries.

a)



b)

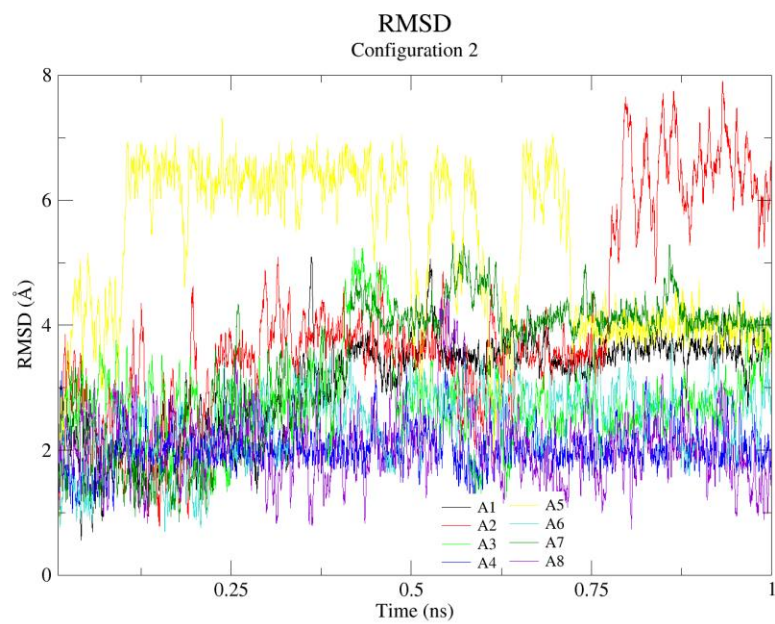
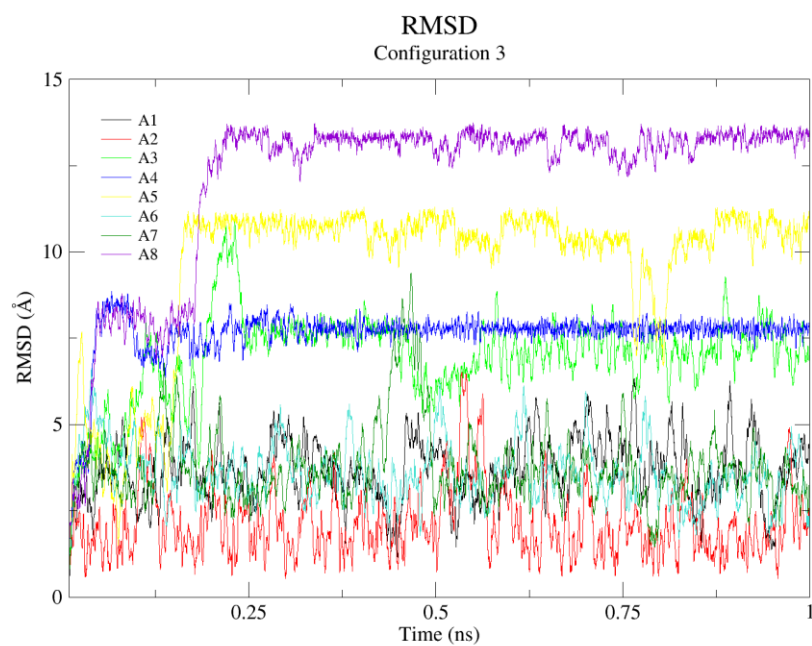


Figure S19 Root Main Square Deviation (RMSD) (Å) values obtained for Conf1 and Conf2 for all the dyes.

a)



b)

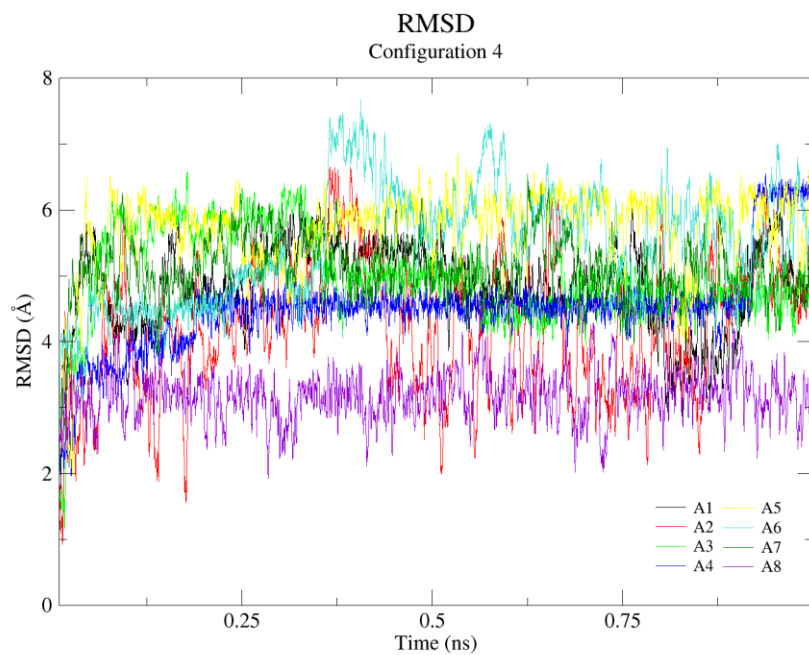
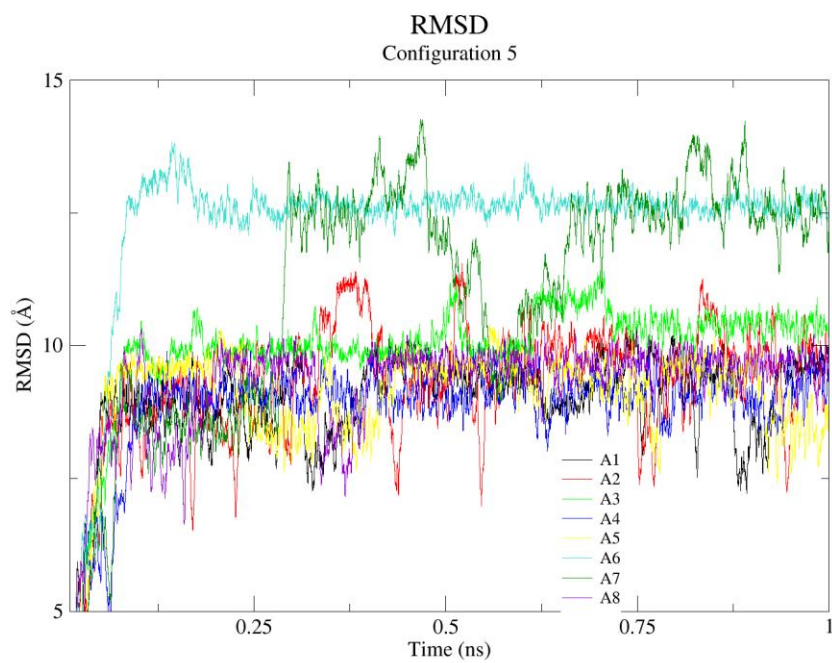


Figure S20 Root Main Square Deviation (RMSD) (Å) values obtained for Conf3 and Conf4 for all the dyes.

a)



b)

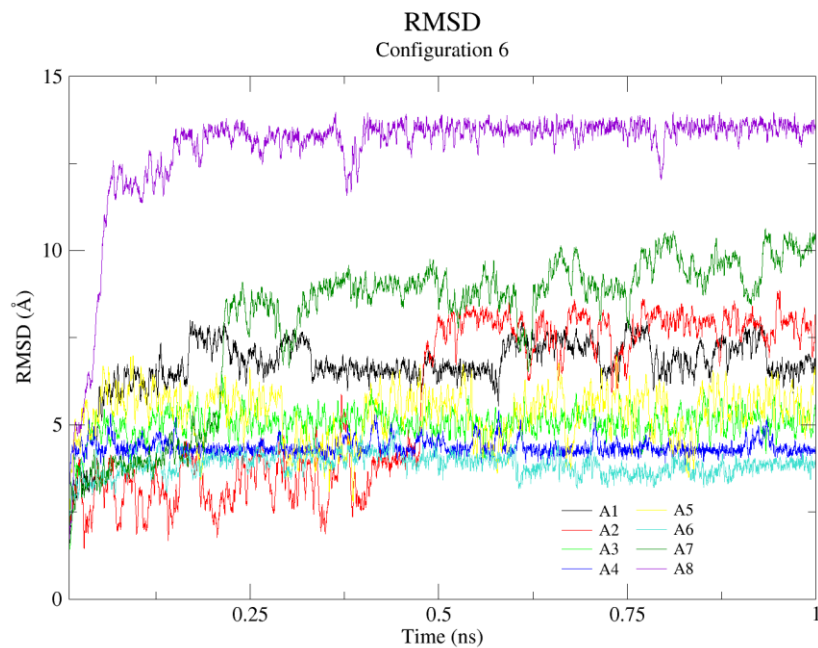


Figure S21 Root Main Square Deviation (RMSD) (Å) values obtained for Conf5 and Conf6 for all the dyes.

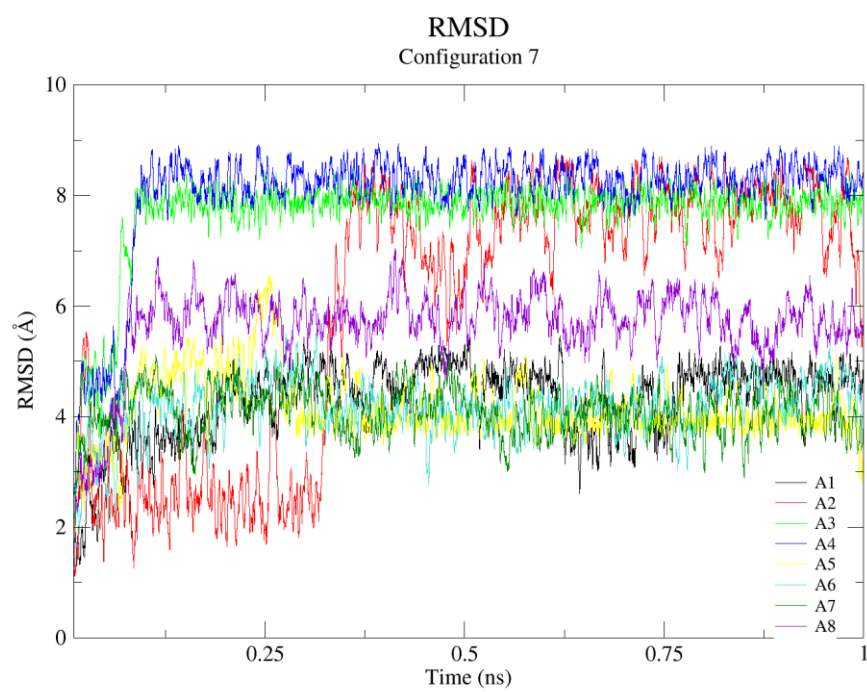


Figure S22 Root Mean Square Deviation (RMSD) (Å) values obtained for Conf7 for all the dyes.

Cartesian coordinates of the optimized ground state dyes
using B3LYP

A1

C	2.420897000	-0.080995000	-0.018153000
C	1.790951000	-1.180123000	-0.635047000
C	1.605165000	0.900933000	0.577441000
H	2.394763000	-1.940195000	-1.118806000
H	2.063914000	1.749165000	1.073548000
C	0.409206000	-1.290221000	-0.649175000
C	0.223784000	0.784944000	0.553384000
H	-0.041457000	-2.133535000	-1.163692000
H	-0.370914000	1.546787000	1.050625000
C	-0.415202000	-0.312645000	-0.055946000
N	3.823533000	0.034160000	0.000326000
C	4.648248000	-1.127919000	0.065357000
C	5.770361000	-1.243598000	-0.768554000
C	4.358466000	-2.158948000	0.972190000
C	6.587798000	-2.369828000	-0.690763000
C	5.171729000	-3.289401000	1.030616000
C	6.291744000	-3.400386000	0.203822000
H	5.996237000	-0.448508000	-1.472115000
H	3.497818000	-2.067820000	1.627451000
H	7.453770000	-2.445811000	-1.342883000
H	4.935310000	-4.079814000	1.737961000
H	6.927468000	-4.279467000	0.257440000
C	4.445014000	1.317900000	-0.045802000
C	4.025423000	2.279065000	-0.977984000
C	5.493591000	1.626312000	0.833289000
C	4.638255000	3.530310000	-1.017495000
C	6.112341000	2.873959000	0.774806000
C	5.686238000	3.833756000	-0.145727000
H	3.221851000	2.039564000	-1.667515000
H	5.818000000	0.884882000	1.556684000
H	4.303444000	4.265173000	-1.744692000
H	6.923548000	3.099464000	1.461817000
H	6.166579000	4.807198000	-0.184479000
C	-2.617992000	-1.601475000	-0.282881000
C	-1.867138000	-0.448649000	-0.079160000
S	-2.923241000	0.917727000	0.155011000
C	-4.369891000	-0.076376000	-0.004402000
C	-4.007096000	-1.399485000	-0.242400000
H	-2.166437000	-2.576268000	-0.426860000
H	-4.731714000	-2.194008000	-0.368938000
C	-5.641399000	0.555350000	0.120123000
H	-5.639695000	1.624239000	0.325891000
C	-6.900668000	0.022123000	0.018322000
C	-7.151913000	-1.354311000	-0.247267000
N	-7.321492000	-2.486443000	-0.465056000
C	-8.048083000	0.946191000	0.198095000
O	-7.952806000	2.136300000	0.428492000
O	-9.238872000	0.315278000	0.076728000
H	-9.920477000	0.999803000	0.209624000

A2

C	3.067464000	-0.126648000	-0.030960000
C	2.572954000	-1.269786000	-0.685119000

C	2.145781000	0.733940000	0.590801000
H	3.263659000	-1.937582000	-1.188063000
H	2.504587000	1.614129000	1.112616000
C	1.211994000	-1.539506000	-0.709763000
C	0.785171000	0.459294000	0.556879000
H	0.858212000	-2.410507000	-1.252482000
H	0.102920000	1.128787000	1.072812000
C	0.281014000	-0.684901000	-0.088439000
N	4.453823000	0.149583000	-0.002681000
C	5.395224000	-0.912739000	0.112904000
C	6.549539000	-0.926319000	-0.685373000
C	5.187187000	-1.954289000	1.030725000
C	7.477570000	-1.958046000	-0.559330000
C	6.112070000	-2.991146000	1.136474000
C	7.263756000	-2.998233000	0.347133000
H	6.712625000	-0.125536000	-1.398850000
H	4.301084000	-1.944453000	1.656603000
H	8.366154000	-1.953903000	-1.184012000
H	5.936993000	-3.789623000	1.851774000
H	7.985769000	-3.803804000	0.437808000
C	4.922306000	1.492127000	-0.080763000
C	4.366318000	2.389921000	-1.005595000
C	5.954234000	1.932463000	0.762479000
C	4.828695000	3.702581000	-1.073842000
C	6.422287000	3.241888000	0.673963000
C	5.860972000	4.136175000	-0.239463000
H	3.574160000	2.053014000	-1.665858000
H	6.384316000	1.243817000	1.481932000
H	4.387951000	4.384930000	-1.794941000
H	7.221670000	3.566914000	1.333650000
H	6.223447000	5.157580000	-0.300842000
C	-1.761168000	-2.222195000	-0.256862000
C	-1.148542000	-0.993773000	-0.119032000
S	-2.360711000	0.265846000	0.006815000
C	-3.680934000	-0.885379000	-0.104812000
C	-3.176272000	-2.160635000	-0.249904000
H	-1.205424000	-3.150355000	-0.321442000
H	-3.807834000	-3.039421000	-0.309717000
C	-5.078906000	-0.459869000	-0.045607000
C	-6.098062000	-1.285483000	-0.565722000
C	-5.453900000	0.771825000	0.526687000
C	-7.428589000	-0.900890000	-0.503027000
C	-6.785487000	1.163409000	0.580098000
C	-7.788306000	0.328177000	0.068811000
H	-5.836216000	-2.225087000	-1.040491000
H	-4.693279000	1.420151000	0.950807000
H	-8.211566000	-1.535208000	-0.904405000
H	-7.055491000	2.113615000	1.026215000
C	-9.224655000	0.692568000	0.102861000
O	-10.129879000	0.004315000	-0.328332000
O	-9.455100000	1.902743000	0.676836000
H	-10.417571000	2.028273000	0.641361000

A3

C	3.990337000	-0.234933000	-0.039128000
C	3.741823000	-1.442488000	-0.720258000
C	2.903923000	0.413986000	0.578085000
H	4.557758000	-1.950936000	-1.221300000

H	3.071204000	1.336798000	1.121690000
C	2.463203000	-1.975637000	-0.773916000
C	1.627308000	-0.123208000	0.513277000
H	2.302019000	-2.889387000	-1.337082000
H	0.819319000	0.390086000	1.026263000
C	1.369007000	-1.333427000	-0.160059000
N	5.287913000	0.310934000	0.021208000
C	6.432984000	-0.536366000	0.067766000
C	7.554778000	-0.250982000	-0.725168000
C	6.459974000	-1.655389000	0.914524000
C	8.681470000	-1.068664000	-0.665800000
C	7.584598000	-2.477138000	0.953650000
C	8.702436000	-2.187934000	0.168468000
H	7.536856000	0.611753000	-1.382565000
H	5.599627000	-1.873758000	1.538287000
H	9.542219000	-0.834811000	-1.285537000
H	7.591175000	-3.339211000	1.614351000
H	9.579611000	-2.826220000	0.207685000
C	5.474798000	1.725371000	0.034654000
C	4.791986000	2.542219000	-0.879092000
C	6.354211000	2.312182000	0.956323000
C	4.979683000	3.922922000	-0.859427000
C	6.548819000	3.692118000	0.956994000
C	5.860568000	4.505068000	0.054280000
H	4.118231000	2.089622000	-1.599083000
H	6.880131000	1.681872000	1.665683000
H	4.444680000	4.543767000	-1.572066000
H	7.232586000	4.133776000	1.676005000
H	6.009472000	5.580324000	0.062119000
C	-0.316483000	-3.231517000	-0.477454000
C	0.029568000	-1.909474000	-0.228433000
S	-1.393578000	-0.922449000	0.004236000
C	-2.461426000	-2.305378000	-0.216966000
C	-1.701071000	-3.447729000	-0.470444000
H	0.412623000	-4.018657000	-0.626466000
H	-2.161798000	-4.416561000	-0.632624000
C	-3.887601000	-2.352779000	-0.171373000
H	-4.254557000	-3.361217000	-0.362134000
C	-7.088100000	-0.188901000	0.388959000
S	-6.590123000	-1.845243000	0.031754000
C	-4.862383000	-1.422501000	0.053136000
C	-4.706865000	0.002780000	0.338514000
O	-3.665964000	0.638725000	0.432298000
S	-8.661486000	0.285721000	0.538303000
N	-5.972086000	0.605050000	0.519497000
C	-6.054557000	2.030162000	0.785967000
C	-6.365486000	2.899001000	-0.426513000
O	-6.657568000	4.067368000	-0.334300000
O	-6.235028000	2.242386000	-1.595803000
H	-6.445074000	2.884928000	-2.294587000
H	-5.078624000	2.338188000	1.170270000
H	-6.821804000	2.223281000	1.536540000
A4			
C	3.714996000	-0.260378000	-0.018130000
C	3.249369000	-1.562482000	-0.336463000
C	2.746506000	0.724743000	0.308313000
H	3.961302000	-2.330785000	-0.610862000

H	3.070676000	1.721200000	0.580978000
C	1.902510000	-1.854012000	-0.330630000
C	1.403064000	0.418217000	0.315029000
H	1.591117000	-2.852013000	-0.619855000
H	0.700399000	1.193154000	0.609022000
C	0.929160000	-0.876925000	-0.004707000
N	5.064837000	0.037367000	-0.022165000
C	6.056962000	-0.994638000	0.099498000
C	7.083810000	-1.085847000	-0.847447000
C	6.019626000	-1.884863000	1.180555000
C	8.063202000	-2.068595000	-0.713760000
C	6.997360000	-2.871472000	1.299816000
C	8.021502000	-2.965754000	0.355484000
H	7.110385000	-0.388446000	-1.678145000
H	5.232751000	-1.796253000	1.922845000
H	8.856984000	-2.136060000	-1.451065000
H	6.966156000	-3.557179000	2.140844000
H	8.785395000	-3.730207000	0.454991000
C	5.532790000	1.389058000	-0.149237000
C	5.108975000	2.185831000	-1.220991000
C	6.446044000	1.897630000	0.781965000
C	5.586190000	3.489746000	-1.346384000
C	6.926090000	3.198621000	0.641975000
C	6.495923000	3.999568000	-0.417972000
H	4.417891000	1.779374000	-1.952565000
H	6.776578000	1.272504000	1.604823000
H	5.258080000	4.101496000	-2.181072000
H	7.634037000	3.588013000	1.366891000
H	6.871860000	5.012216000	-0.523115000
C	-1.071030000	-2.470628000	-0.071635000
C	-0.471564000	-1.203816000	-0.009953000
S	-1.704784000	0.037949000	0.041389000
C	-3.011372000	-1.154748000	0.034448000
C	-2.459150000	-2.442762000	-0.053929000
H	-0.498729000	-3.388709000	-0.090304000
H	-3.068730000	-3.339719000	-0.059098000
C	-8.233464000	-1.258226000	-0.558170000
C	-6.883625000	-1.011291000	-0.315212000
C	-6.450285000	0.201346000	0.238080000
C	-7.368414000	1.209242000	0.546197000
C	-8.716761000	0.963146000	0.300035000
C	-9.147387000	-0.255415000	-0.242628000
C	-4.395777000	-0.874717000	0.008209000
N	-5.057746000	0.231851000	0.437975000
H	-8.561395000	-2.199652000	-0.984978000
H	-7.053750000	2.162546000	0.954413000
H	-9.444018000	1.734033000	0.530514000
H	-10.203646000	-0.419704000	-0.425798000
S	-5.511696000	-2.055069000	-0.652957000
C	-4.442899000	1.355820000	1.132878000
C	-4.125561000	2.506651000	0.176486000
O	-4.078633000	2.403421000	-1.023609000
O	-3.888422000	3.627923000	0.874973000
H	-3.656809000	4.330013000	0.241544000
H	-3.521632000	1.029547000	1.619620000
H	-5.115169000	1.694974000	1.923558000

A5

C	2.708839000	-0.143805000	-0.047804000	H	-6.014148000	-2.041202000	0.824619000
C	2.212408000	-1.204134000	-0.825942000	H	-5.208127000	1.842022000	-0.848205000
C	1.790760000	0.639113000	0.671636000	C	-3.961580000	-1.593078000	0.414401000
H	2.901673000	-1.809204000	-1.404960000	C	-3.508634000	0.587102000	-0.498313000
H	2.152194000	1.455811000	1.286899000	H	-3.624634000	-2.550375000	0.798737000
C	0.851076000	-1.471501000	-0.874384000	H	-2.821421000	1.328408000	-0.895849000
C	0.429568000	0.368344000	0.613741000	C	-3.018157000	-0.656236000	-0.054199000
H	0.495981000	-2.276053000	-1.510656000	N	-7.177223000	0.239492000	0.016622000
H	-0.249900000	0.975204000	1.205289000	C	-8.146724000	-0.782298000	-0.204192000
C	-0.077936000	-0.695887000	-0.154206000	C	-9.273325000	-0.877986000	0.627216000
N	4.098325000	0.128952000	0.006310000	C	-7.994443000	-1.695144000	-1.259746000
C	5.034416000	-0.941371000	0.053874000	C	-10.230142000	-1.866486000	0.400904000
C	6.209558000	-0.892877000	-0.712997000	C	-8.947372000	-2.691433000	-1.467738000
C	4.798694000	-2.059928000	0.869195000	C	-10.071491000	-2.781277000	-0.642910000
C	7.129517000	-1.937631000	-0.655009000	H	-9.393669000	-0.178049000	1.447362000
C	5.716004000	-3.108039000	0.905836000	H	-7.131661000	-1.618414000	-1.913041000
C	6.888189000	-3.053199000	0.149225000	H	-11.096574000	-1.928183000	1.052783000
H	6.394636000	-0.034281000	-1.349658000	H	-8.816356000	-3.390269000	-2.288664000
H	3.896576000	-2.100625000	1.470292000	H	-10.815129000	-3.553632000	-0.812558000
H	8.033726000	-1.883750000	-1.254588000	C	-7.622593000	1.569415000	0.277405000
H	5.518255000	-3.965682000	1.542497000	C	-7.074591000	2.310371000	1.336030000
H	7.604051000	-3.868471000	0.186048000	C	-8.625254000	2.146201000	-0.516956000
C	4.562583000	1.473724000	0.025353000	C	-7.516580000	3.609059000	1.584680000
C	3.990261000	2.437854000	-0.819827000	C	-9.073583000	3.439282000	-0.250328000
C	5.602372000	1.855530000	0.888018000	C	-8.519854000	4.179482000	0.797179000
C	4.444511000	3.754711000	-0.791960000	H	-6.306696000	1.864763000	1.959575000
C	6.061921000	3.170852000	0.895164000	H	-9.047651000	1.578222000	-1.339227000
C	5.484701000	4.129856000	0.060616000	H	-7.084107000	4.170554000	2.407547000
H	3.191277000	2.148533000	-1.494232000	H	-9.850230000	3.873061000	-0.873278000
H	6.044933000	1.117004000	1.547881000	H	-8.866662000	5.188271000	0.998198000
H	3.990474000	4.487692000	-1.452704000	C	-0.988810000	-2.223408000	-0.051788000
H	6.867265000	3.448911000	1.569031000	C	-1.593224000	-0.979450000	-0.070956000
H	5.840599000	5.155335000	0.074328000	S	-0.371762000	0.277346000	-0.100769000
C	-2.121987000	-2.199141000	-0.510305000	C	0.940946000	-0.892525000	-0.103716000
C	-1.508068000	-1.003130000	-0.208745000	C	0.423322000	-2.173905000	-0.068941000
S	-2.724745000	0.217530000	0.128399000	H	-1.549083000	-3.150610000	-0.058855000
C	-4.044067000	-0.906608000	-0.147762000	H	1.043518000	-3.062217000	-0.089442000
C	-3.539842000	-2.144427000	-0.478591000	C	2.337516000	-0.477403000	-0.135028000
H	-1.567005000	-3.103371000	-0.732663000	C	3.354446000	-1.375799000	0.194400000
H	-4.174929000	-2.991097000	-0.713060000	C	2.699148000	0.857537000	-0.503542000
C	-5.444310000	-0.496699000	-0.008296000	H	3.132765000	-2.390113000	0.504677000
C	-6.428286000	-1.428714000	0.351090000	H	1.921077000	1.563594000	-0.774281000
C	-5.846233000	0.834928000	-0.232171000	C	4.703209000	-0.984815000	0.155147000
H	-6.149692000	-2.454799000	0.564120000	C	4.009181000	1.260722000	-0.541317000
H	-5.109457000	1.575219000	-0.536372000	H	4.262495000	2.276737000	-0.827701000
C	-7.762336000	-1.040528000	0.469340000	C	5.052371000	0.351471000	-0.215185000
C	-7.173206000	1.229826000	-0.104075000	C	6.910150000	-1.536656000	0.458244000
H	-8.514891000	-1.773176000	0.753762000	C	7.404163000	-0.228001000	0.100002000
C	-8.152693000	0.279086000	0.248943000	C	6.412727000	0.697377000	-0.235076000
O	-7.599698000	2.508649000	-0.316824000	H	6.684404000	1.707526000	-0.515408000
H	-6.836577000	3.054830000	-0.546860000	N	5.669262000	-1.900852000	0.488043000
O	-9.440052000	0.717832000	0.356776000	Cl	8.066825000	-2.809118000	0.907778000
H	-10.002035000	-0.030253000	0.597704000	C	8.820799000	0.054117000	0.107770000
A6				H	9.460252000	-0.766367000	0.415944000
C	-5.799603000	-0.059309000	-0.009603000	C	9.524825000	1.180696000	-0.206072000
C	-5.318279000	-1.304837000	0.439026000	C	8.963318000	2.414596000	-0.648259000
C	-4.864627000	0.881512000	-0.481420000	N	8.514539000	3.426978000	-1.010679000
				C	11.012170000	1.112107000	-0.078076000

O	11.625791000	0.128211000	0.287620000
O	11.600500000	2.273032000	-0.416882000
H	12.560867000	2.158464000	-0.310914000

A7

C	-5.575025000	-0.050733000	-0.002237000
C	-5.111576000	-1.284076000	0.494000000
C	-4.628543000	0.856719000	-0.512683000
H	-5.819479000	-1.991510000	0.910887000
H	-4.961587000	1.807263000	-0.913772000
C	-3.759671000	-1.593476000	0.475027000
C	-3.277554000	0.540530000	-0.523470000
H	-3.431744000	-2.537661000	0.898450000
H	-2.578191000	1.251908000	-0.953332000
C	-2.805042000	-0.691933000	-0.034844000
N	-6.949263000	0.268095000	0.015329000
C	-7.929873000	-0.747156000	-0.181062000
C	-9.064371000	-0.803120000	0.642667000
C	-7.779929000	-1.695438000	-1.204840000
C	-10.029735000	-1.787366000	0.440045000
C	-8.741941000	-2.686745000	-1.388196000
C	-9.873116000	-2.737203000	-0.571197000
H	-9.182880000	-0.073597000	1.436812000
H	-6.910076000	-1.648929000	-1.851589000
H	-10.902546000	-1.818024000	1.085754000
H	-8.612428000	-3.413506000	-2.184940000
H	-10.624171000	-3.506346000	-0.721982000
C	-7.375682000	1.610454000	0.236307000
C	-6.802415000	2.381614000	1.259063000
C	-8.383938000	2.171622000	-0.561678000
C	-7.224547000	3.693087000	1.467806000
C	-8.811861000	3.478095000	-0.333823000
C	-8.232843000	4.247760000	0.677014000
H	-6.029350000	1.947804000	1.884481000
H	-8.826597000	1.578735000	-1.355089000
H	-6.772017000	4.278100000	2.263198000
H	-9.593401000	3.899428000	-0.959371000
H	-8.564131000	5.267381000	0.847357000
C	-0.804903000	-2.293729000	-0.043976000
C	-1.385847000	-1.040083000	-0.050784000
S	-0.142372000	0.193449000	-0.062457000
C	1.147572000	-0.997351000	-0.080990000
C	0.608770000	-2.268793000	-0.059418000
H	-1.384680000	-3.208734000	-0.068878000
H	1.215633000	-3.166068000	-0.099138000
C	2.551410000	-0.603874000	-0.113674000
C	3.544980000	-1.502281000	0.301128000
C	2.943598000	0.684929000	-0.564786000
H	3.269924000	-2.479573000	0.684681000
H	2.188310000	1.384563000	-0.906100000
C	4.893801000	-1.141377000	0.256453000
C	4.272704000	1.045647000	-0.600233000
H	4.562290000	2.031636000	-0.951693000
C	5.285557000	0.147019000	-0.195377000
C	7.258050000	-1.755619000	0.667277000
C	7.648711000	-0.406212000	0.188182000
C	6.668973000	0.476144000	-0.216491000
H	6.941348000	1.465384000	-0.567474000

N	5.886917000	-2.008299000	0.658742000
H	5.640592000	-2.933541000	0.988865000
C	9.070992000	-0.161086000	0.202787000
C	9.801338000	0.935310000	-0.154726000
C	9.240776000	2.149207000	-0.653286000
N	8.755182000	3.128059000	-1.058106000
C	11.283798000	0.851897000	-0.011674000
O	11.888817000	-0.116836000	0.397008000
O	11.894685000	1.996030000	-0.394346000
H	12.846767000	1.849608000	-0.267673000
O	8.036642000	-2.620109000	1.051683000
H	9.659639000	-1.001464000	0.563466000

A8

C	6.370985000	0.175193000	0.013011000
C	5.544371000	1.168343000	0.573472000
C	5.754321000	-0.935619000	-0.593347000
H	5.994515000	2.023816000	1.064113000
H	6.367246000	-1.706741000	-1.045960000
C	4.163638000	1.054080000	0.522685000
C	4.372180000	-1.044623000	-0.633674000
H	3.557843000	1.820310000	0.995854000
H	3.931139000	-1.900527000	-1.136623000
C	3.537509000	-0.053752000	-0.082265000
N	7.774691000	0.291252000	0.059831000
C	8.396067000	1.572798000	-0.014372000
C	9.434599000	1.905966000	0.867804000
C	7.986161000	2.509300000	-0.975649000
C	10.052431000	3.152212000	0.783615000
C	8.597820000	3.759723000	-1.040426000
C	9.635594000	4.087387000	-0.165664000
H	9.751676000	1.184364000	1.613245000
H	7.190993000	2.251180000	-1.667228000
H	10.855297000	3.396480000	1.473047000
H	8.270625000	4.474671000	-1.789726000
H	10.114919000	5.059605000	-0.224238000
C	8.595953000	-0.868396000	0.177788000
C	8.278838000	-1.877122000	1.100438000
C	9.741242000	-1.005779000	-0.620629000
C	9.088279000	-3.006192000	1.209158000
C	10.554388000	-2.130045000	-0.491852000
C	10.231412000	-3.138256000	0.418317000
H	7.399747000	-1.769984000	1.727119000
H	9.987944000	-0.228794000	-1.336391000
H	8.830422000	-3.778897000	1.927541000
H	11.437975000	-2.222632000	-1.116594000
H	10.863496000	-4.015835000	0.511429000
C	1.148715000	0.869278000	-0.037431000
C	2.081974000	-0.152906000	-0.128073000
S	1.269664000	-1.688082000	-0.306035000
C	-0.322549000	-0.937952000	-0.276071000
C	-0.188598000	0.436662000	-0.119382000
H	1.429777000	1.911572000	0.053671000
H	-1.029057000	1.118412000	-0.078557000
C	-1.476529000	-1.770950000	-0.402922000
C	-3.825070000	-2.460403000	-0.539729000
C	-2.794256000	-1.429419000	-0.395513000
S	-3.508829000	0.176661000	-0.228767000

C	-5.153108000	-0.497543000	-0.352287000
O	-3.662938000	-3.663004000	-0.671349000
N	-5.109456000	-1.866310000	-0.519459000
C	-6.255334000	-2.758826000	-0.600072000
C	-6.941014000	-3.087606000	0.721512000
O	-7.969836000	-3.716786000	0.778980000
O	-6.265327000	-2.632593000	1.794263000
H	-6.774704000	-2.905823000	2.576446000
C	-8.481308000	1.580770000	-0.187957000
S	-7.979624000	-0.108691000	-0.385634000
C	-6.254328000	0.315309000	-0.292180000
C	-6.114813000	1.756626000	-0.113282000
S	-10.070720000	2.032811000	-0.169479000
N	-7.376508000	2.381739000	-0.072672000
O	-5.065512000	2.384295000	-0.008416000
C	-7.454882000	3.839106000	0.115807000
H	-6.565148000	4.251351000	-0.363769000
H	-8.346351000	4.178521000	-0.414109000
C	-7.506617000	4.230830000	1.591740000
H	-6.611232000	3.885564000	2.115423000
H	-8.390914000	3.810025000	2.076938000
H	-7.554627000	5.320670000	1.678965000
H	-7.004459000	-2.389165000	-1.301464000
H	-5.867741000	-3.702754000	-0.995121000
H	-1.307884000	-2.839825000	-0.522503000

Cartesian coordinates of the ground state dyes using CAM-B3LYP

A1

C	2.406780000	-0.084526000	0.000081000
C	1.779559000	-1.186801000	-0.598171000
C	1.598741000	0.897376000	0.590008000
H	2.379785000	-1.951434000	-1.076056000
H	2.057574000	1.751533000	1.072714000
C	0.401757000	-1.299886000	-0.601568000
C	0.221128000	0.779665000	0.575804000
H	-0.051382000	-2.150608000	-1.098622000
H	-0.371030000	1.547013000	1.064739000
C	-0.411195000	-0.320391000	-0.016372000
N	3.804407000	0.034608000	0.005770000
C	4.632869000	-1.121076000	0.037758000
C	5.724573000	-1.223089000	-0.826524000
C	4.376519000	-2.154038000	0.942120000
C	6.548844000	-2.340225000	-0.781063000
C	5.194442000	-3.276335000	0.968944000
C	6.286196000	-3.374025000	0.111944000
H	5.923806000	-0.422710000	-1.530511000
H	3.535637000	-2.072895000	1.622031000
H	7.394945000	-2.406368000	-1.457253000
H	4.983730000	-4.072491000	1.675500000
H	6.927689000	-4.248194000	0.140941000
C	4.422184000	1.315782000	-0.028320000
C	4.003484000	2.281045000	-0.946604000
C	5.467187000	1.612187000	0.848595000
C	4.614477000	3.528073000	-0.974596000
C	6.085933000	2.855030000	0.802022000

C	5.660402000	3.820384000	-0.104841000
H	3.199029000	2.049572000	-1.636010000
H	5.791339000	0.863884000	1.563407000
H	4.279110000	4.270023000	-1.691900000
H	6.898075000	3.072512000	1.488029000
H	6.140871000	4.792394000	-0.134660000
C	-2.605520000	-1.616671000	-0.169360000
C	-1.866772000	-0.458069000	-0.032066000
S	-2.908876000	0.911305000	0.116301000
C	-4.344514000	-0.078079000	0.008724000
C	-3.993652000	-1.406763000	-0.147414000
H	-2.153467000	-2.596029000	-0.256904000
H	-4.716958000	-2.206279000	-0.229938000
C	-5.617531000	0.560048000	0.088708000
H	-5.613201000	1.637418000	0.236074000
C	-6.867646000	0.030559000	0.006077000
C	-7.128561000	-1.356361000	-0.189579000
N	-7.325854000	-2.486953000	-0.348891000
C	-8.019515000	0.952937000	0.124773000
O	-7.924373000	2.149783000	0.292785000
O	-9.192859000	0.316163000	0.025189000
H	-9.896538000	0.980113000	0.111169000

A2

C	3.052792000	-0.126063000	-0.024939000
C	2.559429000	-1.269109000	-0.665694000
C	2.139174000	0.734070000	0.594105000
H	3.246720000	-1.940944000	-1.166342000
H	2.498115000	1.618727000	1.106687000
C	1.202458000	-1.540702000	-0.680208000
C	0.782161000	0.458605000	0.569867000
H	0.847257000	-2.419042000	-1.208459000
H	0.102981000	1.133730000	1.081044000
C	0.282162000	-0.685291000	-0.062027000
N	4.434529000	0.150761000	-0.006535000
C	5.376001000	-0.907720000	0.094093000
C	6.512000000	-0.918532000	-0.718837000
C	5.183888000	-1.944070000	1.011228000
C	7.440899000	-1.945259000	-0.608593000
C	6.107771000	-2.977122000	1.102191000
C	7.242721000	-2.982211000	0.297456000
H	6.662809000	-0.118071000	-1.434618000
H	4.308200000	-1.935926000	1.650706000
H	8.319291000	-1.939395000	-1.245836000
H	5.944456000	-3.775945000	1.818349000
H	7.966316000	-3.786410000	0.376244000
C	4.900780000	1.489932000	-0.078501000
C	4.345960000	2.387149000	-0.994772000
C	5.929144000	1.923248000	0.761939000
C	4.805910000	3.696118000	-1.057578000
C	6.396596000	3.228590000	0.679757000
C	5.835684000	4.123811000	-0.225347000
H	3.553455000	2.053962000	-1.655616000
H	6.360001000	1.231751000	1.477427000
H	4.364120000	4.381638000	-1.773532000
H	7.196965000	3.549844000	1.338475000
H	6.197879000	5.144626000	-0.282329000
C	-1.752204000	-2.223122000	-0.182560000

C	-1.150475000	-0.997055000	-0.081867000
S	-2.352972000	0.257856000	0.008191000
C	-3.662665000	-0.888373000	-0.074000000
C	-3.169342000	-2.161074000	-0.179229000
H	-1.196076000	-3.151327000	-0.226282000
H	-3.801885000	-3.039259000	-0.219745000
C	-5.063798000	-0.459508000	-0.031488000
C	-6.067840000	-1.280839000	-0.565286000
C	-5.436991000	0.765183000	0.537698000
C	-7.394866000	-0.894645000	-0.518243000
C	-6.764786000	1.157890000	0.575303000
C	-7.755168000	0.327843000	0.050143000
H	-5.801258000	-2.220527000	-1.035174000
H	-4.681637000	1.412309000	0.970734000
H	-8.170150000	-1.529557000	-0.931195000
H	-7.037157000	2.107079000	1.020354000
C	-9.188775000	0.699690000	0.069550000
O	-10.084221000	0.011251000	-0.375430000
O	-9.419375000	1.894421000	0.636241000
H	-10.377504000	2.047739000	0.602327000

A3

C	-3.992388000	-0.219753000	0.039757000
C	-3.735496000	-1.414170000	0.727166000
C	-2.921340000	0.422484000	-0.595268000
H	-4.542897000	-1.920522000	1.242269000
H	-3.095142000	1.339604000	-1.144938000
C	-2.459422000	-1.945077000	0.768531000
C	-1.646375000	-0.111664000	-0.542458000
H	-2.289976000	-2.856092000	1.332195000
H	-0.846392000	0.398909000	-1.069179000
C	-1.383846000	-1.308604000	0.135176000
N	-5.288174000	0.319540000	-0.010016000
C	-6.428088000	-0.529598000	-0.017357000
C	-7.523822000	-0.238019000	0.797748000
C	-6.473027000	-1.652244000	-0.847383000
C	-8.646916000	-1.055123000	0.777065000
C	-7.592087000	-2.474876000	-0.848584000
C	-8.686000000	-2.179557000	-0.041113000
H	-7.490420000	0.631462000	1.444852000
H	-5.628661000	-1.876406000	-1.489741000
H	-9.491685000	-0.815944000	1.414802000
H	-7.613108000	-3.344507000	-1.497334000
H	-9.561621000	-2.819651000	-0.050362000
C	-5.482246000	1.727427000	-0.065658000
C	-4.799102000	2.572218000	0.811894000
C	-6.370902000	2.276381000	-0.992066000
C	-4.995117000	3.945968000	0.751938000
C	-6.575571000	3.649700000	-1.033790000
C	-5.886292000	4.491548000	-0.166878000
H	-4.115708000	2.147208000	1.538784000
H	-6.899492000	1.621574000	-1.676021000
H	-4.457441000	4.591668000	1.438587000
H	-7.269972000	4.063697000	-1.757628000
H	-6.043046000	5.564135000	-0.206030000
C	0.294012000	-3.211305000	0.387482000
C	-0.041758000	-1.890106000	0.185464000
S	1.369930000	-0.903736000	-0.008970000

C	2.430282000	-2.283656000	0.163503000
C	1.679985000	-3.427908000	0.374361000
H	-0.436339000	-4.000151000	0.511874000
H	2.140495000	-4.400655000	0.502392000
C	3.858246000	-2.340526000	0.109063000
H	4.216155000	-3.357696000	0.256169000
C	7.039938000	-0.200657000	-0.394044000
S	6.547476000	-1.848353000	-0.099712000
C	4.828876000	-1.414955000	-0.084691000
C	4.683368000	0.018068000	-0.306166000
O	3.655548000	0.667979000	-0.350664000
S	8.615731000	0.274883000	-0.536661000
N	5.948167000	0.611867000	-0.481382000
C	6.052067000	2.037279000	-0.706506000
C	6.509896000	2.828055000	0.502624000
O	6.946435000	3.949883000	0.420474000
O	6.328010000	2.174334000	1.651101000
H	6.621335000	2.754341000	2.373847000
H	5.054051000	2.387970000	-0.978302000
H	6.738519000	2.240962000	-1.527117000

A4

C	3.681034000	-0.262146000	-0.022230000
C	3.218276000	-1.526200000	-0.421576000
C	2.735776000	0.685929000	0.398705000
H	3.923636000	-2.270932000	-0.768571000
H	3.065159000	1.663184000	0.728726000
C	1.870319000	-1.825647000	-0.395972000
C	1.388780000	0.379143000	0.416521000
H	1.545401000	-2.801388000	-0.740051000
H	0.691109000	1.128337000	0.777901000
C	0.922655000	-0.881785000	0.023027000
N	5.045118000	0.043600000	-0.043930000
C	6.026068000	-0.974913000	0.125010000
C	7.111173000	-1.049431000	-0.749363000
C	5.924844000	-1.890481000	1.174186000
C	8.082775000	-2.026427000	-0.572493000
C	6.890722000	-2.875860000	1.333947000
C	7.975258000	-2.946600000	0.465249000
H	7.189154000	-0.338347000	-1.564418000
H	5.088530000	-1.826057000	1.861584000
H	8.922720000	-2.073879000	-1.257757000
H	6.801138000	-3.582847000	2.152178000
H	8.732115000	-3.712241000	0.597466000
C	5.489783000	1.383839000	-0.231367000
C	4.987447000	2.157405000	-1.279303000
C	6.450934000	1.925125000	0.623252000
C	5.433343000	3.460751000	-1.458048000
C	6.905142000	3.223312000	0.427658000
C	6.395936000	3.998398000	-0.609250000
H	4.248934000	1.733144000	-1.950670000
H	6.839805000	1.323314000	1.437298000
H	5.035474000	4.053403000	-2.275244000
H	7.653872000	3.633444000	1.097379000
H	6.748018000	5.013749000	-0.756297000
C	-1.071563000	-2.473202000	0.116703000
C	-0.496431000	-1.221020000	0.043553000
S	-1.708238000	0.010975000	-0.056907000

C	-2.993868000	-1.164418000	0.044129000
C	-2.473141000	-2.443483000	0.105954000
H	-0.495791000	-3.383943000	0.210478000
H	-3.091823000	-3.329029000	0.187232000
C	-8.164330000	-1.151329000	-0.798021000
C	-6.827636000	-0.943344000	-0.472706000
C	-6.419002000	0.196279000	0.218130000
C	-7.337392000	1.174517000	0.593687000
C	-8.665974000	0.967322000	0.265600000
C	-9.077419000	-0.182127000	-0.419834000
C	-4.392319000	-0.865832000	-0.032697000
N	-5.037727000	0.190540000	0.470243000
H	-8.475365000	-2.040668000	-1.332583000
H	-7.035607000	2.071717000	1.119033000
H	-9.400022000	1.713727000	0.545421000
H	-10.125462000	-0.314200000	-0.661966000
S	-5.454019000	-1.948646000	-0.849123000
C	-4.426253000	1.228447000	1.287711000
C	-4.034871000	2.430309000	0.445960000
O	-3.944124000	2.408603000	-0.756119000
O	-3.783496000	3.478540000	1.220502000
H	-3.493490000	4.217881000	0.658893000
H	-3.538942000	0.830939000	1.781485000
H	-5.123621000	1.518130000	2.072969000

A5

C	2.695362000	-0.147001000	-0.033764000
C	2.198021000	-1.212981000	-0.792148000
C	1.786440000	0.638934000	0.681771000
H	2.882111000	-1.824913000	-1.368557000
H	2.149069000	1.463606000	1.284154000
C	0.840807000	-1.483669000	-0.825817000
C	0.429042000	0.365961000	0.637743000
H	0.482577000	-2.299929000	-1.443944000
H	-0.246306000	0.981611000	1.223677000
C	-0.075820000	-0.703068000	-0.110683000
N	4.078786000	0.129159000	0.004952000
C	5.019998000	-0.932884000	0.015977000
C	6.170822000	-0.863655000	-0.773591000
C	4.812376000	-2.057670000	0.818862000
C	7.097401000	-1.898021000	-0.752198000
C	5.734161000	-3.096492000	0.819664000
C	6.883366000	-3.022168000	0.039000000
H	6.334746000	0.004553000	-1.402100000
H	3.925857000	-2.113824000	1.440624000
H	7.986756000	-1.828483000	-1.370243000
H	5.557640000	-3.963845000	1.447590000
H	7.605186000	-3.831739000	0.047672000
C	4.538862000	1.471315000	0.045452000
C	3.971329000	2.441099000	-0.785297000
C	5.570088000	1.838141000	0.913849000
C	4.421700000	3.753975000	-0.737102000
C	6.027870000	3.149164000	0.942326000
C	5.454442000	4.115622000	0.122249000
H	3.176084000	2.160957000	-1.467141000
H	6.010656000	1.090698000	1.564162000
H	3.969733000	4.495763000	-1.387656000
H	6.830487000	3.417922000	1.621537000

H	5.809080000	5.140244000	0.152116000
C	-2.112095000	-2.217630000	-0.393450000
C	-1.508990000	-1.013908000	-0.150772000
S	-2.715474000	0.215597000	0.117699000
C	-4.025472000	-0.912425000	-0.103732000
C	-3.531782000	-2.159791000	-0.369105000
H	-1.556125000	-3.129850000	-0.572554000
H	-4.167607000	-3.016391000	-0.557057000
C	-5.428002000	-0.493425000	0.013479000
C	-6.402288000	-1.397399000	0.436160000
C	-5.824063000	0.815090000	-0.298298000
H	-6.122923000	-2.408075000	0.710283000
H	-5.091847000	1.536815000	-0.649430000
C	-7.733393000	-1.006436000	0.533458000
C	-7.146884000	1.211519000	-0.192915000
H	-8.484315000	-1.716851000	0.867116000
C	-8.119467000	0.290072000	0.225732000
O	-7.576363000	2.467931000	-0.488639000
H	-6.822971000	3.007208000	-0.761876000
O	-9.401398000	0.736309000	0.306864000
H	-9.972707000	0.013337000	0.596867000

A6

C	-5.762154000	-0.048849000	-0.000711000
C	-5.269658000	-1.245019000	0.535407000
C	-4.853156000	0.840688000	-0.584452000
H	-5.952674000	-1.941367000	1.007449000
H	-5.211981000	1.767108000	-1.017030000
C	-3.918308000	-1.538653000	0.484177000
C	-3.501623000	0.542439000	-0.626442000
H	-3.562998000	-2.459716000	0.933640000
H	-2.827084000	1.243261000	-1.108356000
C	-3.002857000	-0.653613000	-0.098493000
N	-7.137760000	0.251520000	0.049015000
C	-8.102374000	-0.781767000	-0.089883000
C	-9.206058000	-0.833961000	0.764776000
C	-7.964624000	-1.751560000	-1.086120000
C	-10.156831000	-1.835876000	0.618375000
C	-8.909717000	-2.761272000	-1.213933000
C	-10.012437000	-2.807472000	-0.366819000
H	-9.314730000	-0.085469000	1.541797000
H	-7.114500000	-1.710129000	-1.758000000
H	-11.009635000	-1.862868000	1.288936000
H	-8.788777000	-3.508433000	-1.991612000
H	-10.752821000	-3.592868000	-0.474119000
C	-7.575646000	1.588718000	0.240183000
C	-6.969356000	2.404662000	1.198857000
C	-8.627478000	2.100453000	-0.523565000
C	-7.402108000	3.712094000	1.378402000
C	-9.067072000	3.402905000	-0.324591000
C	-8.455058000	4.217726000	0.622425000
H	-6.158564000	2.009583000	1.800678000
H	-9.098279000	1.472005000	-1.271289000
H	-6.920538000	4.334178000	2.125917000
H	-9.886194000	3.785856000	-0.924636000
H	-8.795807000	5.236766000	0.770611000
C	-0.993199000	-2.227972000	-0.148786000
C	-1.576292000	-0.987855000	-0.147742000

S	-0.356935000	0.251493000	-0.195238000
C	0.934303000	-0.917778000	-0.230321000
C	0.422624000	-2.187875000	-0.194822000
H	-1.563832000	-3.148227000	-0.149796000
H	1.041499000	-3.075758000	-0.235377000
C	2.339832000	-0.511233000	-0.283542000
C	3.331387000	-1.365498000	0.161353000
C	2.709373000	0.764491000	-0.797783000
H	3.094491000	-2.333585000	0.585644000
H	1.937918000	1.434613000	-1.160851000
C	4.685002000	-0.990632000	0.095622000
C	4.017824000	1.150841000	-0.861693000
H	4.285542000	2.123769000	-1.259959000
C	5.043042000	0.281248000	-0.415910000
C	6.872868000	-1.524497000	0.477910000
C	7.370109000	-0.271251000	-0.011070000
C	6.408826000	0.614100000	-0.458144000
H	6.696329000	1.574194000	-0.869066000
N	5.632955000	-1.869620000	0.539873000
Cl	8.019088000	-2.714621000	1.082685000
C	8.797783000	-0.007552000	-0.065049000
H	9.450601000	-0.874237000	-0.067870000
C	9.456110000	1.169721000	-0.103135000
C	8.832057000	2.454166000	-0.035296000
N	8.329707000	3.495316000	0.022310000
C	10.944731000	1.126461000	-0.185310000
O	11.589561000	0.104663000	-0.240148000
O	11.482558000	2.348008000	-0.188653000
H	12.448060000	2.250936000	-0.239783000

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C	-5.551950000	-0.048888000	-0.008267000
C	-5.084874000	-1.268317000	0.497787000
C	-4.620158000	0.847532000	-0.543948000
H	-5.785558000	-1.971164000	0.932721000
H	-4.958554000	1.792094000	-0.953036000
C	-3.736377000	-1.577110000	0.464468000
C	-3.271897000	0.533711000	-0.568167000
H	-3.401827000	-2.516885000	0.890507000
H	-2.579345000	1.241438000	-1.013019000
C	-2.798345000	-0.685033000	-0.069523000
N	-6.923766000	0.268461000	0.024118000
C	-7.900633000	-0.747114000	-0.154386000
C	-9.017520000	-0.803798000	0.682558000
C	-7.762002000	-1.694067000	-1.172236000
C	-9.980347000	-1.787706000	0.497793000
C	-8.719591000	-2.686262000	-1.338583000
C	-9.835304000	-2.736892000	-0.508879000
H	-9.126884000	-0.073129000	1.476264000
H	-6.901478000	-1.648521000	-1.830488000
H	-10.843345000	-1.818478000	1.155012000
H	-8.597984000	-3.415817000	-2.132696000
H	-10.585276000	-3.508364000	-0.646357000
C	-7.347405000	1.606151000	0.244374000
C	-6.754429000	2.383903000	1.242150000
C	-8.372066000	2.155426000	-0.529931000
C	-7.173334000	3.691647000	1.450095000
C	-8.798343000	3.457785000	-0.303107000

C	-8.199289000	4.234850000	0.683174000
H	-5.964911000	1.959011000	1.851924000
H	-8.832042000	1.556057000	-1.307717000
H	-6.702551000	4.284169000	2.227869000
H	-9.596393000	3.870557000	-0.911696000
H	-8.529388000	5.253984000	0.853257000
C	-0.804891000	-2.280278000	-0.121474000
C	-1.374983000	-1.034018000	-0.099986000
S	-0.142532000	0.192845000	-0.091899000
C	1.137065000	-0.988822000	-0.132886000
C	0.611600000	-2.254203000	-0.138815000
H	-1.384602000	-3.194117000	-0.156735000
H	1.220685000	-3.148242000	-0.190891000
C	2.545531000	-0.593172000	-0.155481000
C	3.522048000	-1.482995000	0.281409000
C	2.934153000	0.685018000	-0.619869000
H	3.244384000	-2.455555000	0.671225000
H	2.182298000	1.379414000	-0.976650000
C	4.868085000	-1.120572000	0.245233000
C	4.257747000	1.045778000	-0.644595000
H	4.551042000	2.026106000	-1.005268000
C	5.258191000	0.152618000	-0.215740000
C	7.202674000	-1.732997000	0.688827000
C	7.601814000	-0.396972000	0.201944000
C	6.641266000	0.479983000	-0.223917000
H	6.918406000	1.464033000	-0.583336000
N	5.849909000	-1.986840000	0.669591000
H	5.586797000	-2.906245000	1.003270000
C	9.023573000	-0.156059000	0.232666000
C	9.767327000	0.917039000	-0.126500000
C	9.237596000	2.132435000	-0.655711000
N	8.799332000	3.115169000	-1.084530000
C	11.241641000	0.824836000	0.040058000
O	11.822021000	-0.143695000	0.477004000
O	11.863730000	1.942769000	-0.350959000
H	12.817119000	1.814426000	-0.215879000
O	7.988354000	-2.585873000	1.090148000
H	9.599312000	-0.994055000	0.615086000

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C	6.344873000	0.169199000	0.025546000
C	5.523255000	1.154527000	0.589580000
C	5.733684000	-0.935000000	-0.581810000
H	5.971808000	2.009281000	1.081427000
H	6.345555000	-1.704696000	-1.036555000
C	4.145951000	1.040476000	0.539000000
C	4.354835000	-1.044978000	-0.621783000
H	3.539349000	1.807023000	1.008893000
H	3.915396000	-1.901169000	-1.124104000
C	3.528360000	-0.060060000	-0.068657000
N	7.744637000	0.288286000	0.069288000
C	8.361105000	1.567578000	0.000553000
C	9.396756000	1.894836000	0.878178000
C	7.949134000	2.503990000	-0.950473000
C	10.012517000	3.137459000	0.799470000
C	8.556867000	3.751452000	-1.010507000
C	9.593530000	4.073781000	-0.140340000
H	9.716040000	1.170374000	1.619203000

H	7.152030000	2.249879000	-1.640392000
H	10.817077000	3.378101000	1.486729000
H	8.226105000	4.470018000	-1.753363000
H	10.071492000	5.045941000	-0.195065000
C	8.567606000	-0.866537000	0.164539000
C	8.268454000	-1.878478000	1.079901000
C	9.695269000	-0.993041000	-0.649402000
C	9.079595000	-3.002541000	1.167380000
C	10.512014000	-2.111479000	-0.542847000
C	10.207028000	-3.123925000	0.361099000
H	7.399100000	-1.779519000	1.720432000
H	9.928240000	-0.210432000	-1.362874000
H	8.834818000	-3.781591000	1.882039000
H	11.385913000	-2.195798000	-1.180626000
H	10.842810000	-3.999388000	0.437658000
C	1.150900000	0.867494000	-0.062645000
C	2.068463000	-0.156668000	-0.119938000
S	1.262055000	-1.682898000	-0.260137000
C	-0.314630000	-0.934909000	-0.257807000
C	-0.187981000	0.433142000	-0.139336000
H	1.434404000	1.909874000	0.005317000
H	-1.024898000	1.118725000	-0.120822000
C	-1.474840000	-1.769744000	-0.371625000
C	-3.812515000	-2.451999000	-0.507707000
C	-2.778387000	-1.423977000	-0.379181000
S	-3.491205000	0.178770000	-0.248497000
C	-5.123053000	-0.494275000	-0.365385000
O	-3.648887000	-3.652252000	-0.607987000
N	-5.084524000	-1.860991000	-0.508897000
C	-6.234147000	-2.738765000	-0.594581000
C	-6.932939000	-3.020535000	0.722362000
O	-7.981775000	-3.613458000	0.781008000
O	-6.256606000	-2.569987000	1.778497000
H	-6.757603000	-2.803586000	2.578378000
C	-8.434737000	1.546739000	-0.191032000
S	-7.937818000	-0.121265000	-0.391836000
C	-6.222621000	0.308928000	-0.313863000
C	-6.092031000	1.745741000	-0.146838000
S	-10.030677000	1.985416000	-0.149910000
N	-7.353831000	2.359843000	-0.094616000
O	-5.053602000	2.381965000	-0.056301000
C	-7.441348000	3.812164000	0.090457000
H	-6.568138000	4.232405000	-0.408321000
H	-8.340230000	4.146069000	-0.426714000
C	-7.467706000	4.199018000	1.561320000
H	-6.560932000	3.859964000	2.066794000
H	-8.335255000	3.767572000	2.064894000
H	-7.524067000	5.286235000	1.651356000
H	-6.961225000	-2.378593000	-1.321707000
H	-5.857241000	-3.695048000	-0.964287000
H	-1.304791000	-2.839800000	-0.466156000

Cartesian coordinates of the ground state dyes using
BHandHLYP

A1

C	2.400978000	-0.083209000	-0.000866000
C	1.774613000	-1.186538000	-0.588724000

C	1.594494000	0.900691000	0.578255000
H	2.369508000	-1.950592000	-1.057058000
H	2.048874000	1.752898000	1.051628000
C	0.401697000	-1.298525000	-0.592466000
C	0.221673000	0.784189000	0.563663000
H	-0.046246000	-2.147663000	-1.080313000
H	-0.364679000	1.551381000	1.042942000
C	-0.410120000	-0.316940000	-0.017996000
N	3.792212000	0.034352000	0.005250000
C	4.617800000	-1.117597000	0.040120000
C	5.684704000	-1.237973000	-0.844915000
C	4.384038000	-2.128181000	0.968441000
C	6.507154000	-2.351045000	-0.796683000
C	5.199593000	-3.246747000	0.999084000
C	6.266829000	-3.362490000	0.120912000
H	5.866428000	-0.458048000	-1.565029000
H	3.565468000	-2.033628000	1.661935000
H	7.330938000	-2.431388000	-1.486836000
H	5.007459000	-4.022531000	1.722015000
H	6.904398000	-4.230262000	0.152437000
C	4.410266000	1.310069000	-0.030659000
C	4.017978000	2.259633000	-0.969763000
C	5.429651000	1.616862000	0.865177000
C	4.629601000	3.501462000	-1.000344000
C	6.049480000	2.854348000	0.817096000
C	5.650151000	3.803909000	-0.111209000
H	3.236285000	2.021494000	-1.671334000
H	5.732761000	0.883951000	1.593799000
H	4.316279000	4.228407000	-1.731619000
H	6.838676000	3.079260000	1.515638000
H	6.129603000	4.768110000	-0.142576000
C	-2.596459000	-1.607811000	-0.177440000
C	-1.860116000	-0.452898000	-0.034286000
S	-2.902276000	0.910295000	0.121197000
C	-4.333979000	-0.078308000	0.009222000
C	-3.979851000	-1.400783000	-0.154034000
H	-2.148144000	-2.580205000	-0.269875000
H	-4.694999000	-2.197309000	-0.239897000
C	-5.602932000	0.553929000	0.093414000
H	-5.595882000	1.622165000	0.248274000
C	-6.851714000	0.028809000	0.006542000
C	-7.113091000	-1.352691000	-0.200789000
N	-7.311607000	-2.473506000	-0.368998000
C	-7.997531000	0.947320000	0.132307000
O	-7.900891000	2.134870000	0.309387000
O	-9.165083000	0.320785000	0.028243000
H	-9.866187000	0.971177000	0.117546000

A2

C	3.045972000	-0.125468000	-0.024844000
C	2.552087000	-1.261192000	-0.668865000
C	2.135649000	0.729434000	0.596226000
H	3.232948000	-1.927149000	-1.170036000
H	2.491993000	1.605399000	1.109808000
C	1.199446000	-1.530654000	-0.684442000
C	0.782668000	0.456687000	0.570993000
H	0.847354000	-2.400058000	-1.214114000
H	0.110364000	1.126203000	1.082613000

C	0.282077000	-0.680215000	-0.063937000
N	4.422438000	0.148955000	-0.005712000
C	5.360190000	-0.905952000	0.096396000
C	6.480741000	-0.930935000	-0.729703000
C	5.180744000	-1.925331000	1.028117000
C	7.406774000	-1.954332000	-0.618465000
C	6.101372000	-2.955328000	1.120861000
C	7.220891000	-2.974266000	0.302519000
H	6.622224000	-0.147063000	-1.454474000
H	4.320518000	-1.907240000	1.675773000
H	8.269808000	-1.959408000	-1.264026000
H	5.948449000	-3.737766000	1.846123000
H	7.939398000	-3.772983000	0.382119000
C	4.888488000	1.482927000	-0.078519000
C	4.357248000	2.368757000	-1.012718000
C	5.893450000	1.923193000	0.778761000
C	4.817117000	3.673073000	-1.077194000
C	6.361357000	3.223775000	0.695826000
C	5.823821000	4.107422000	-0.227775000
H	3.585679000	2.032148000	-1.684397000
H	6.305097000	1.243733000	1.505786000
H	4.395454000	4.347041000	-1.804927000
H	7.140520000	3.549250000	1.365599000
H	6.184904000	5.120727000	-0.285551000
C	-1.747118000	-2.209346000	-0.189666000
C	-1.146312000	-0.989104000	-0.084965000
S	-2.346781000	0.262375000	0.008540000
C	-3.654207000	-0.880971000	-0.077363000
C	-3.160723000	-2.147506000	-0.186543000
H	-1.196660000	-3.132267000	-0.236130000
H	-3.786829000	-3.021137000	-0.230002000
C	-5.051357000	-0.456303000	-0.033173000
C	-6.052575000	-1.277293000	-0.563490000
C	-5.425203000	0.764747000	0.533501000
C	-7.375436000	-0.894549000	-0.515081000
C	-6.749417000	1.153409000	0.572568000
C	-7.736870000	0.324353000	0.051310000
H	-5.788493000	-2.210332000	-1.030496000
H	-4.676885000	1.410061000	0.962333000
H	-8.142458000	-1.528651000	-0.924767000
H	-7.018771000	2.096171000	1.014769000
C	-9.165361000	0.694336000	0.073313000
O	-10.054248000	0.008708000	-0.367057000
O	-9.396234000	1.880230000	0.635399000
H	-10.342412000	2.040921000	0.608712000

A3

C	-3.979900000	-0.224888000	0.034038000
C	-3.722786000	-1.419504000	0.712584000
C	-2.911383000	0.419281000	-0.593947000
H	-4.523988000	-1.926887000	1.220540000
H	-3.083049000	1.332832000	-1.135412000
C	-2.450594000	-1.947168000	0.753299000
C	-1.640102000	-0.111441000	-0.541883000
H	-2.284126000	-2.854301000	1.309481000
H	-0.846750000	0.401008000	-1.061174000
C	-1.376743000	-1.308045000	0.127921000
N	-5.270062000	0.312351000	-0.013159000

C	-6.406973000	-0.532372000	-0.025756000
C	-7.489420000	-0.259451000	0.805538000
C	-6.463216000	-1.632425000	-0.877476000
C	-8.610314000	-1.072136000	0.779682000
C	-7.579760000	-2.451103000	-0.884637000
C	-8.660394000	-2.174001000	-0.060663000
H	-7.448715000	0.589087000	1.467417000
H	-5.632686000	-1.842204000	-1.530155000
H	-9.441510000	-0.848216000	1.428097000
H	-7.609345000	-3.299762000	-1.548261000
H	-9.530992000	-2.808332000	-0.074250000
C	-5.463070000	1.716065000	-0.056418000
C	-4.809955000	2.546856000	0.849560000
C	-6.320749000	2.275184000	-0.998715000
C	-5.004966000	3.916902000	0.802842000
C	-6.524907000	3.644596000	-1.028364000
C	-5.865537000	4.472404000	-0.132333000
H	-4.152656000	2.116036000	1.586021000
H	-6.824614000	1.634308000	-1.702524000
H	-4.492916000	4.549289000	1.509463000
H	-7.192645000	4.065072000	-1.762360000
H	-6.021238000	5.537979000	-0.161495000
C	0.300930000	-3.197012000	0.395300000
C	-0.037910000	-1.883243000	0.181434000
S	1.369433000	-0.898785000	-0.021566000
C	2.430512000	-2.271215000	0.166491000
C	1.683344000	-3.409824000	0.386626000
H	-0.420987000	-3.982424000	0.526220000
H	2.140517000	-4.374482000	0.525443000
C	3.853345000	-2.327564000	0.123097000
H	4.207648000	-3.335253000	0.286966000
C	7.032878000	-0.206896000	-0.696688000
S	6.537730000	-1.842633000	-0.059148000
C	4.824267000	-1.408623000	-0.074107000
C	4.687285000	0.016236000	-0.320607000
O	3.669417000	0.663939000	-0.389246000
S	8.610807000	0.260804000	-0.492105000
N	5.949260000	0.601073000	-0.488046000
C	6.057404000	2.017552000	-0.741657000
C	6.432978000	2.843315000	0.466360000
O	6.827526000	3.971152000	0.373726000
O	6.236088000	2.213649000	1.613589000
H	6.472950000	2.805070000	2.333476000
H	5.085503000	2.356150000	-1.082328000
H	6.787836000	2.202086000	-1.517425000

A4

C	3.674488000	-0.260656000	-0.018544000
C	3.211646000	-1.522972000	-0.409656000
C	2.731630000	0.687244000	0.395154000
H	3.910866000	-2.265817000	-0.749524000
H	3.058092000	1.659359000	0.718477000
C	1.868331000	-1.819770000	-0.384616000
C	1.389235000	0.382911000	0.412885000
H	1.547405000	-2.790592000	-0.722349000
H	0.698216000	1.130546000	0.767479000
C	0.922339000	-0.875818000	0.026287000
N	5.032278000	0.042631000	-0.041271000

C	6.009810000	-0.973027000	0.125593000
C	7.069226000	-1.072489000	-0.770021000
C	5.931067000	-1.860773000	1.194268000
C	8.037945000	-2.046662000	-0.595159000
C	6.893637000	-2.843431000	1.353251000
C	7.952679000	-2.938909000	0.462851000
H	7.130335000	-0.385747000	-1.597435000
H	5.117871000	-1.777540000	1.895593000
H	8.854928000	-2.113575000	-1.294661000
H	6.822140000	-3.525951000	2.184099000
H	8.704457000	-3.699344000	0.593491000
C	5.477533000	1.377261000	-0.231123000
C	5.001196000	2.136173000	-1.295700000
C	6.413837000	1.927900000	0.637360000
C	5.448071000	3.434083000	-1.477885000
C	6.869319000	3.220721000	0.439414000
C	6.385959000	3.980937000	-0.614725000
H	4.284579000	1.706955000	-1.975644000
H	6.782014000	1.340341000	1.461508000
H	5.072090000	4.012955000	-2.305410000
H	7.595912000	3.636699000	1.117831000
H	6.737735000	4.988224000	-0.763479000
C	-1.066400000	-2.460344000	0.098026000
C	-0.491367000	-1.211300000	0.043277000
S	-1.701927000	0.018048000	-0.038085000
C	-2.985760000	-1.156273000	0.044015000
C	-2.462711000	-2.430745000	0.086878000
H	-0.496517000	-3.367240000	0.178235000
H	-3.074329000	-3.313370000	0.153790000
C	-8.142011000	-1.165503000	-0.782505000
C	-6.809799000	-0.951340000	-0.464395000
C	-6.401373000	0.193181000	0.208777000
C	-7.318718000	1.169941000	0.573715000
C	-8.644204000	0.956974000	0.253189000
C	-9.054251000	-0.196991000	-0.414941000
C	-4.378912000	-0.862698000	-0.029805000
N	-5.024431000	0.194085000	0.457005000
H	-8.450537000	-2.055804000	-1.301685000
H	-7.021762000	2.068083000	1.084452000
H	-9.373506000	1.700291000	0.524777000
H	-10.095438000	-0.333317000	-0.650960000
S	-5.437899000	-1.955426000	-0.830966000
C	-4.421293000	1.233071000	1.270974000
C	-4.040212000	2.439233000	0.440401000
O	-4.000844000	2.443673000	-0.755774000
O	-3.739785000	3.458636000	1.220591000
H	-3.466808000	4.205320000	0.679136000
H	-3.539033000	0.845815000	1.764985000
H	-5.117026000	1.516722000	2.050006000

A5

C	2.689401000	-0.145070000	-0.033993000
C	2.191882000	-1.202500000	-0.796240000
C	1.783608000	0.633849000	0.684328000
H	2.869815000	-1.807350000	-1.373422000
H	2.143356000	1.448966000	1.288063000
C	0.839067000	-1.471364000	-0.831298000
C	0.430277000	0.363257000	0.639204000

H	0.484239000	-2.277712000	-1.451205000
H	-0.238382000	0.972112000	1.225932000
C	-0.074882000	-0.697348000	-0.113278000
N	4.067661000	0.128565000	0.005219000
C	5.004065000	-0.931213000	0.018972000
C	6.135820000	-0.880189000	-0.791096000
C	4.811327000	-2.035854000	0.845181000
C	7.058414000	-1.912305000	-0.767322000
C	5.728703000	-3.072827000	0.849394000
C	6.858967000	-3.016346000	0.047785000
H	6.288393000	-0.030943000	-1.435433000
H	3.942920000	-2.078387000	1.480573000
H	7.929640000	-1.857288000	-1.399483000
H	5.564556000	-3.921199000	1.493598000
H	7.574843000	-3.821283000	0.058713000
C	4.528955000	1.464877000	0.043935000
C	3.980159000	2.427750000	-0.799805000
C	5.543878000	1.833960000	0.923207000
C	4.432465000	3.735442000	-0.753958000
C	6.004028000	3.139627000	0.949972000
C	5.449031000	4.099004000	0.116623000
H	3.200415000	2.148094000	-1.487943000
H	5.969211000	1.095501000	1.581520000
H	3.996654000	4.468844000	-1.412651000
H	6.790901000	3.408839000	1.635575000
H	5.804030000	5.115710000	0.144760000
C	-2.105883000	-2.202034000	-0.404662000
C	-1.503819000	-1.005430000	-0.155098000
S	-2.708678000	0.219158000	0.120433000
C	-4.015996000	-0.905130000	-0.108014000
C	-3.522244000	-2.144759000	-0.380611000
H	-1.555515000	-3.107991000	-0.588768000
H	-4.151558000	-2.995901000	-0.573399000
C	-5.414994000	-0.490855000	0.011032000
C	-6.385528000	-1.395384000	0.426966000
C	-5.812967000	0.814648000	-0.291752000
H	-6.108669000	-2.400508000	0.694297000
H	-5.087584000	1.535108000	-0.636043000
C	-7.712407000	-1.007434000	0.525615000
C	-7.131853000	1.207318000	-0.184822000
H	-8.456652000	-1.716352000	0.852975000
C	-8.099525000	0.285809000	0.226488000
O	-7.557317000	2.459484000	-0.472773000
H	-6.816596000	3.001121000	-0.739156000
O	-9.376731000	0.723917000	0.310925000
H	-9.946100000	0.009946000	0.592306000

A6

C	-5.748198000	-0.050419000	-0.000713000
C	-5.255423000	-1.241407000	0.535608000
C	-4.841970000	0.836787000	-0.581690000
H	-5.932474000	-1.934087000	1.004530000
H	-5.198080000	1.756025000	-1.013169000
C	-3.908119000	-1.532092000	0.487127000
C	-3.494260000	0.541957000	-0.621088000
H	-3.556100000	-2.445815000	0.936011000
H	-2.826177000	1.239442000	-1.099818000
C	-2.995050000	-0.649154000	-0.093179000

N	-7.118600000	0.247408000	0.046618000	C	-5.070704000	-1.263962000	0.500610000
C	-8.080075000	-0.780666000	-0.099282000	C	-4.608943000	0.844433000	-0.538699000
C	-9.172767000	-0.847136000	0.761068000	H	-5.765428000	-1.963267000	0.932211000
C	-7.951673000	-1.731665000	-1.108526000	H	-4.944599000	1.781618000	-0.947246000
C	-10.121477000	-1.844042000	0.608011000	C	-3.726235000	-1.569514000	0.471036000
C	-8.894470000	-2.736590000	-1.243717000	C	-3.264471000	0.534281000	-0.559304000
C	-9.986113000	-2.796773000	-0.390458000	H	-3.395083000	-2.501825000	0.896956000
H	-9.275075000	-0.116524000	1.545585000	H	-2.578415000	1.238801000	-1.000862000
H	-7.113710000	-1.680161000	-1.783018000	C	-2.790451000	-0.679427000	-0.060175000
H	-10.962403000	-1.881865000	1.281067000	N	-6.904802000	0.264132000	0.022176000
H	-8.781080000	-3.466022000	-2.028997000	C	-7.877452000	-0.747203000	-0.162746000
H	-10.722084000	-3.575376000	-0.502886000	C	-8.983227000	-0.819507000	0.680104000
C	-7.555556000	1.579159000	0.242792000	C	-7.747118000	-1.674675000	-1.193362000
C	-6.978110000	2.375712000	1.228430000	C	-9.942922000	-1.799230000	0.489145000
C	-8.577517000	2.105091000	-0.542968000	C	-8.701324000	-2.662867000	-1.366680000
C	-7.409601000	3.678186000	1.413621000	C	-9.805856000	-2.728895000	-0.530575000
C	-9.016522000	3.402492000	-0.339493000	H	-9.086990000	-0.107011000	1.480929000
C	-8.433004000	4.197875000	0.635096000	H	-6.898837000	-1.617894000	-1.854412000
H	-6.193266000	1.971422000	1.845065000	H	-10.793975000	-1.841951000	1.149039000
H	-9.024573000	1.494348000	-1.309019000	H	-8.586525000	-3.374252000	-2.168138000
H	-6.952516000	4.282926000	2.179749000	H	-10.550553000	-3.494232000	-0.672699000
H	-9.809319000	3.795400000	-0.954860000	C	-7.329096000	1.596310000	0.243996000
H	-8.771811000	5.209195000	0.786652000	C	-6.767575000	2.357139000	1.266224000
C	-0.989103000	-2.213792000	-0.136922000	C	-8.322873000	2.157373000	-0.553317000
C	-1.572520000	-0.979469000	-0.139750000	C	-7.186950000	3.659777000	1.476481000
S	-0.356303000	0.257563000	-0.189311000	C	-8.750256000	3.454609000	-0.325332000
C	0.933780000	-0.908060000	-0.220410000	C	-8.182455000	4.214587000	0.686119000
C	0.422935000	-2.172803000	-0.181677000	H	-6.004605000	1.925161000	1.891507000
H	-1.553217000	-3.129453000	-0.136230000	H	-8.757083000	1.573880000	-1.347525000
H	1.036243000	-3.055752000	-0.219196000	H	-6.742649000	4.236918000	2.270880000
C	2.334574000	-0.504311000	-0.274957000	H	-9.521293000	3.875246000	-0.949934000
C	3.323829000	-1.356356000	0.168581000	H	-8.511991000	5.225904000	0.856930000
C	2.702973000	0.767870000	-0.789103000	C	-0.800829000	-2.265196000	-0.101255000
H	3.088020000	-2.316852000	0.591302000	C	-1.371199000	-1.024380000	-0.087162000
H	1.937498000	1.433792000	-1.149684000	S	-0.141982000	0.200213000	-0.084730000
C	4.672395000	-0.983356000	0.101323000	C	1.136438000	-0.978064000	-0.118603000
C	4.006824000	1.152084000	-0.854665000	C	0.611611000	-2.238306000	-0.117504000
H	4.271806000	2.117868000	-1.251670000	H	-1.373972000	-3.174640000	-0.131957000
C	5.029025000	0.284839000	-0.410203000	H	1.214995000	-3.127619000	-0.163968000
C	6.851674000	-1.517357000	0.480416000	C	2.539897000	-0.585827000	-0.144558000
C	7.348592000	-0.267794000	-0.007692000	C	3.515038000	-1.475250000	0.286719000
C	6.389667000	0.615734000	-0.453232000	C	2.927046000	0.689799000	-0.606217000
H	6.675211000	1.568387000	-0.862325000	H	3.239910000	-2.441252000	0.673347000
N	5.616972000	-1.857411000	0.542853000	H	2.180867000	1.381329000	-0.957206000
Cl	7.988977000	-2.706137000	1.082650000	C	4.855836000	-1.115539000	0.247346000
C	8.771586000	-0.007557000	-0.063784000	C	4.246124000	1.047707000	-0.634550000
H	9.415524000	-0.870767000	-0.059860000	H	4.536354000	2.021650000	-0.992348000
C	9.434780000	1.162744000	-0.111294000	C	5.244067000	0.155040000	-0.211556000
C	8.818534000	2.447375000	-0.049585000	C	7.180365000	-1.727625000	0.681354000
N	8.325338000	3.484110000	0.003614000	C	7.581048000	-0.396719000	0.197915000
C	10.916926000	1.111924000	-0.194503000	C	6.621610000	0.479518000	-0.222833000
O	11.551443000	0.092911000	-0.245490000	H	6.896667000	1.456838000	-0.578623000
O	11.460419000	2.320374000	-0.203456000	N	5.834899000	-1.978835000	0.665564000
H	12.415555000	2.227997000	-0.254414000	H	5.573470000	-2.890792000	0.995326000
				C	8.997830000	-0.157117000	0.225173000
				C	9.742874000	0.911643000	-0.133033000
				C	9.216562000	2.125804000	-0.658988000
				N	8.784538000	3.103767000	-1.083175000
A7							
C	-5.538112000	-0.049871000	-0.006378000				

C	11.210849000	0.815742000	0.030592000
O	11.784587000	-0.148864000	0.463325000
O	11.834395000	1.922539000	-0.356712000
H	12.778511000	1.800947000	-0.227521000
O	7.960539000	-2.577227000	1.076706000
H	9.569439000	-0.989525000	0.602565000

A8

C	6.330338000	0.169349000	0.025688000
C	5.511795000	1.151814000	0.589032000
C	5.718711000	-0.930915000	-0.578558000
H	5.957261000	2.000664000	1.077380000
H	6.324160000	-1.696178000	-1.031529000
C	4.139123000	1.039210000	0.540435000
C	4.344375000	-1.040035000	-0.616224000
H	3.539386000	1.801469000	1.008714000
H	3.908347000	-1.890577000	-1.114771000
C	3.520807000	-0.057725000	-0.064236000
N	7.724236000	0.286954000	0.067382000
C	8.340668000	1.560876000	0.000249000
C	9.356388000	1.893676000	0.891627000
C	7.949459000	2.486912000	-0.962949000
C	9.972998000	3.131221000	0.814945000
C	8.557638000	3.729391000	-1.021843000
C	9.574458000	4.057029000	-0.137449000
H	9.659170000	1.180531000	1.639685000
H	7.170755000	2.230229000	-1.661235000
H	10.758983000	3.375286000	1.510740000
H	8.244324000	4.437105000	-1.771822000
H	10.051179000	5.021617000	-0.190773000
C	8.544256000	-0.864486000	0.158077000
C	8.267938000	-1.858666000	1.092875000
C	9.646933000	-1.005371000	-0.679392000
C	9.076544000	-2.979475000	1.176856000
C	10.461770000	-2.120322000	-0.577315000
C	10.179209000	-3.114972000	0.346567000
H	7.421248000	-1.749550000	1.749412000
H	9.862239000	-0.239621000	-1.405377000
H	8.850569000	-3.741771000	1.904399000
H	11.313049000	-2.215619000	-1.231318000
H	10.810976000	-3.984473000	0.419734000
C	1.152476000	0.868214000	-0.054251000
C	2.065983000	-0.153403000	-0.113163000
S	1.257400000	-1.674005000	-0.252283000
C	-0.314598000	-0.924567000	-0.248496000
C	-0.183243000	0.438051000	-0.129496000
H	1.434265000	1.903418000	0.013520000
H	-1.011502000	1.122475000	-0.109208000
C	-1.472674000	-1.753639000	-0.361136000
C	-3.803678000	-2.432536000	-0.497992000
C	-2.772510000	-1.409351000	-0.372066000
S	-3.485572000	0.187841000	-0.249864000
C	-5.112222000	-0.483716000	-0.365685000
O	-3.641538000	-3.625608000	-0.591167000
N	-5.069336000	-1.845799000	-0.505653000
C	-6.213153000	-2.723573000	-0.601600000
C	-6.896791000	-3.041182000	0.709686000
O	-7.929930000	-3.645946000	0.756152000

O	-6.229783000	-2.609464000	1.766370000
H	-6.710599000	-2.861074000	2.560220000
C	-8.417966000	1.540953000	-0.185072000
S	-7.920384000	-0.118573000	-0.387731000
C	-6.209489000	0.314553000	-0.315530000
C	-6.087949000	1.749488000	-0.150797000
S	-10.013951000	1.969213000	-0.137770000
N	-7.345500000	2.353996000	-0.093635000
O	-5.060535000	2.387223000	-0.065784000
C	-7.438552000	3.803915000	0.087281000
H	-6.584406000	4.226414000	-0.425643000
H	-8.342546000	4.127737000	-0.410625000
C	-7.441203000	4.196457000	1.552683000
H	-6.529397000	3.868358000	2.041204000
H	-8.291700000	3.765126000	2.070444000
H	-7.502751000	5.277242000	1.636180000
H	-6.943511000	-2.349267000	-1.306403000
H	-5.845299000	-3.663709000	-0.996959000
H	-1.302618000	-2.816176000	-0.451341000

Cartesian coordinates of the oxidized dyes using B3LYP

A1+

C	2.411272178	-0.078662736	-0.034612249
C	1.784545156	-1.249573962	-0.539528363
C	1.588268261	0.979718791	0.435616060
H	2.392780947	-2.052779056	-0.937083985
H	2.045145266	1.866405935	0.857443021
C	0.413084949	-1.347776760	-0.575497838
C	0.218079331	0.862758776	0.406392504
H	-0.029667770	-2.238473036	-1.005067307
H	-0.378380222	1.674712180	0.809668348
C	-0.422650189	-0.299792618	-0.100637135
N	3.791969187	0.029956074	-0.001304461
C	4.619216496	-1.130015914	0.104448999
C	5.753349938	-1.248149115	-0.715340906
C	4.311832069	-2.130141922	1.042416727
C	6.564427846	-2.372500102	-0.602730865
C	5.134689854	-3.247527143	1.146053260
C	6.258908948	-3.373391200	0.324893524
H	5.978650539	-0.474100600	-1.440536129
H	3.454397076	-2.013699734	1.696426672
H	7.433397797	-2.471587684	-1.244697461
H	4.906384331	-4.013938521	1.879310044
H	6.897956147	-4.246005092	0.411118219
C	4.428386835	1.307516886	-0.072718209
C	4.018084122	2.243278367	-1.037130924
C	5.478884750	1.608510995	0.809218183
C	4.653809871	3.479291977	-1.105418025
C	6.102519132	2.849432834	0.731226526
C	5.693286521	3.786458552	-0.222852923
H	3.230113343	1.988806246	-1.737841661
H	5.783143253	0.881816512	1.554323255
H	4.347473078	4.197830044	-1.858418988
H	6.905215348	3.088898917	1.420704904
H	6.186753831	4.750996877	-0.281503348
C	-2.615184720	-1.546944027	-0.488625614

C	-1.856063033	-0.422666332	-0.136626774
S	-2.915019137	0.903308797	0.287719606
C	-4.348054490	-0.060108926	-0.005109407
C	-3.994681698	-1.350824673	-0.415269268
H	-2.175189152	-2.492750694	-0.778773044
H	-4.722801593	-2.116466527	-0.647188258
C	-5.625202735	0.556659800	0.194882826
H	-5.633525053	1.593892521	0.523512672
C	-6.870357226	0.020693053	0.030061835
C	-7.107949026	-1.317956368	-0.392517533
N	-7.261521926	-2.418919519	-0.740022690
C	-8.040791571	0.916386323	0.318425159
O	-7.927333640	2.066301302	0.682142833
O	-9.208258184	0.286295436	0.123389695
H	-9.920176742	0.917423823	0.326001828

A2+

C	3.053210000	-0.129132000	-0.050000000
C	2.572368000	-1.390156000	-0.498516000
C	2.101422000	0.854983000	0.333849000
H	3.277289000	-2.143880000	-0.826965000
H	2.443791000	1.810812000	0.710636000
C	1.223000000	-1.642115000	-0.564745000
C	0.754850000	0.585107000	0.276030000
H	0.895119000	-2.600188000	-0.950606000
H	0.060080000	1.347444000	0.613385000
C	0.259411000	-0.668707000	-0.176894000
N	4.408753000	0.133361000	0.011451000
C	5.360582000	-0.924669000	0.168435000
C	6.496445000	-0.961064000	-0.653971000
C	5.170137000	-1.899768000	1.159867000
C	7.428943000	-1.981040000	-0.489431000
C	6.111605000	-2.914051000	1.314225000
C	7.239975000	-2.958818000	0.491508000
H	6.633766000	-0.204084000	-1.418373000
H	4.305546000	-1.845432000	1.812875000
H	8.302419000	-2.015709000	-1.132184000
H	5.970669000	-3.661550000	2.088067000
H	7.972352000	-3.749433000	0.617691000
C	4.907377000	1.472113000	-0.081950000
C	4.451083000	2.322559000	-1.101188000
C	5.875632000	1.915238000	0.831258000
C	4.956636000	3.616725000	-1.192628000
C	6.371838000	3.211425000	0.728701000
C	5.914691000	4.064871000	-0.279710000
H	3.727087000	1.961098000	-1.823796000
H	6.220752000	1.251254000	1.616198000
H	4.612454000	4.270456000	-1.987371000
H	7.112997000	3.557963000	1.441375000
H	6.307988000	5.073184000	-0.356908000
C	-1.773069000	-2.163306000	-0.552302000
C	-1.145097000	-0.950097000	-0.245158000
S	-2.360279000	0.282144000	0.065920000
C	-3.672495000	-0.841552000	-0.202558000
C	-3.167717000	-2.101847000	-0.528805000
H	-1.229079000	-3.075086000	-0.765255000
H	-3.803149000	-2.958546000	-0.713566000
C	-5.064550000	-0.435120000	-0.086848000

C	-6.085535000	-1.238960000	-0.641996000
C	-5.430897000	0.756460000	0.574599000
C	-7.415298000	-0.864207000	-0.533778000
C	-6.762857000	1.131095000	0.680365000
C	-7.764787000	0.321481000	0.127264000
H	-5.832354000	-2.145874000	-1.179538000
H	-4.668669000	1.382015000	1.029034000
H	-8.204823000	-1.472267000	-0.961145000
H	-7.034926000	2.044529000	1.195548000
C	-9.213689000	0.671568000	0.210799000
O	-10.103064000	-0.005365000	-0.259172000
O	-9.433212000	1.830433000	0.869880000
H	-10.395206000	1.970827000	0.871814000

A3+

C	-3.954543000	-0.239464000	0.080607000
C	-3.745072000	-1.567482000	0.544971000
C	-2.816507000	0.532338000	-0.282959000
H	-4.593281000	-2.163333000	0.858250000
H	-2.952111000	1.534610000	-0.669671000
C	-2.474703000	-2.083191000	0.641769000
C	-1.552615000	0.000152000	-0.192418000
H	-2.354356000	-3.085621000	1.035439000
H	-0.712710000	0.607599000	-0.513513000
C	-1.327894000	-1.324692000	0.274711000
N	-5.228077000	0.286152000	-0.016444000
C	-6.369906000	-0.563212000	-0.180197000
C	-7.503944000	-0.358341000	0.619213000
C	-6.362525000	-1.570592000	-1.157234000
C	-8.620172000	-1.171586000	0.446308000
C	-7.486240000	-2.376756000	-1.320079000
C	-8.615076000	-2.181320000	-0.520283000
H	-7.498979000	0.422120000	1.372213000
H	-5.493225000	-1.700800000	-1.793073000
H	-9.494019000	-1.020099000	1.071418000
H	-7.485096000	-3.148391000	-2.082994000
H	-9.489608000	-2.809742000	-0.653087000
C	-5.452241000	1.699865000	0.039186000
C	-4.866023000	2.465234000	1.059006000
C	-6.284013000	2.305701000	-0.913922000
C	-5.104433000	3.836242000	1.111102000
C	-6.513545000	3.676933000	-0.850426000
C	-5.925397000	4.445085000	0.158493000
H	-4.249530000	1.983295000	1.810404000
H	-6.731023000	1.705572000	-1.698904000
H	-4.659780000	4.426730000	1.905478000
H	-7.148421000	4.147770000	-1.593776000
H	-6.110592000	5.513215000	0.204978000
C	0.345724000	-3.195243000	0.714378000
C	-0.007936000	-1.878971000	0.373844000
S	1.422731000	-0.910938000	0.055963000
C	2.479310000	-2.274568000	0.371306000
C	1.716129000	-3.409355000	0.710467000
H	-0.373845000	-3.970966000	0.943434000
H	2.181119000	-4.361265000	0.940544000
C	3.902015000	-2.339256000	0.322154000
H	4.268127000	-3.333198000	0.574377000
C	7.065198000	-0.178301000	-0.436324000

S	6.584505000	-1.823468000	0.044484000
C	4.875683000	-1.421546000	0.024542000
C	4.696131000	-0.004269000	-0.350826000
O	3.634245000	0.591146000	-0.449461000
S	8.625811000	0.274221000	-0.637225000
N	5.934951000	0.595635000	-0.600931000
C	5.995857000	2.011133000	-0.942106000
C	6.222732000	2.948265000	0.240919000
O	6.381500000	4.134578000	0.100145000
O	6.199613000	2.312202000	1.428406000
H	6.359313000	2.987888000	2.110078000
H	5.042085000	2.278947000	-1.401369000
H	6.800233000	2.175891000	-1.660081000

A4+

C	3.725618000	-0.241420000	-0.045070000
C	3.272695000	-1.506659000	-0.476211000
C	2.786328000	0.715822000	0.393461000
H	3.981796000	-2.234950000	-0.852044000
H	3.126117000	1.677322000	0.760123000
C	1.920211000	-1.796778000	-0.474356000
C	1.437119000	0.407340000	0.405337000
H	1.593532000	-2.755731000	-0.859735000
H	0.739715000	1.145056000	0.788984000
C	0.968025000	-0.851737000	-0.029232000
N	5.101237000	0.063409000	-0.055816000
C	6.055597000	-0.932025000	0.264194000
C	7.261943000	-1.001943000	-0.465166000
C	5.803652000	-1.841233000	1.313712000
C	8.197056000	-1.976810000	-0.145590000
C	6.754263000	-2.803241000	1.625520000
C	7.949957000	-2.876864000	0.898607000
H	7.434848000	-0.320549000	-1.290319000
H	4.893125000	-1.756880000	1.896180000
H	9.116139000	-2.045758000	-0.717492000
H	6.574935000	-3.488187000	2.447304000
H	8.687577000	-3.632910000	1.146685000
C	5.539476000	1.367333000	-0.392958000
C	4.913200000	2.073158000	-1.442020000
C	6.611298000	1.948760000	0.317255000
C	5.363832000	3.343615000	-1.773238000
C	7.042110000	3.224382000	-0.021388000
C	6.424671000	3.923970000	-1.065716000
H	4.116797000	1.605693000	-2.010192000
H	7.067643000	1.412486000	1.141504000
H	4.901846000	3.879050000	-2.595770000
H	7.853425000	3.681208000	0.535072000
H	6.770732000	4.917927000	-1.329415000
C	-1.028681000	-2.448611000	-0.079201000
C	-0.454504000	-1.186801000	-0.033376000
S	-1.682347000	0.057559000	-0.017083000
C	-2.964378000	-1.141693000	-0.038899000
C	-2.433976000	-2.424642000	-0.093015000
H	-0.455289000	-3.366929000	-0.071364000
C	-3.048916000	-3.317363000	-0.103150000
C	-8.106740000	-1.021533000	-1.183719000
C	-6.792370000	-0.866645000	-0.738232000
C	-6.450566000	0.116987000	0.204975000

C	-7.419876000	0.986556000	0.719211000
C	-8.725981000	0.831248000	0.271413000
C	-9.067657000	-0.160773000	-0.665256000
C	-4.373695000	-0.843300000	-0.139714000
N	-5.083629000	0.077535000	0.534898000
H	-8.368531000	-1.782203000	-1.910694000
H	-7.172113000	1.763840000	1.432890000
H	-9.496691000	1.492560000	0.651874000
H	-10.097242000	-0.253871000	-0.993222000
S	-5.364375000	-1.755678000	-1.227286000
C	-4.547519000	0.952111000	1.581643000
C	-4.192578000	2.326056000	1.005738000
O	-3.732736000	2.478008000	-0.100632000
O	-4.432697000	3.287415000	1.900016000
H	-4.157674000	4.142924000	1.522338000
H	-3.643633000	0.500149000	1.995684000
H	-5.281578000	1.029247000	2.383750000

A5+

C	2.687871000	-0.152456000	-0.055663000
C	2.205481000	-1.422404000	-0.475186000
C	1.733770000	0.840197000	0.298237000
H	2.910210000	-2.187281000	-0.776927000
H	2.074383000	1.806434000	0.648937000
C	0.855772000	-1.674816000	-0.541276000
C	0.386705000	0.570882000	0.238864000
H	0.530224000	-2.643952000	-0.901185000
H	-0.308100000	1.344464000	0.550431000
C	-0.109254000	-0.692084000	-0.184321000
N	4.042689000	0.109708000	0.006780000
C	4.997708000	-0.947965000	0.164013000
C	6.116490000	-1.001431000	-0.678701000
C	4.828864000	-1.903518000	1.176671000
C	7.054326000	-2.017148000	-0.512302000
C	5.772774000	-2.916390000	1.331293000
C	6.885376000	-2.976933000	0.489089000
H	6.240135000	-0.257070000	-1.457877000
H	3.975283000	-1.838603000	1.843291000
H	7.916263000	-2.061838000	-1.170067000
H	5.645555000	-3.650097000	2.120765000
H	7.620467000	-3.764994000	0.615909000
C	4.544478000	1.449332000	-0.087119000
C	4.121519000	2.287487000	-1.129183000
C	5.485132000	1.903627000	0.847372000
C	4.630738000	3.580837000	-1.221992000
C	5.988953000	3.197459000	0.742139000
C	5.563239000	4.039409000	-0.288719000
H	3.415743000	1.918651000	-1.866161000
H	5.808217000	1.247711000	1.648511000
H	4.309343000	4.225148000	-2.034002000
H	6.711772000	3.550366000	1.470564000
H	5.960950000	5.045935000	-0.367449000
C	-2.141973000	-2.190548000	-0.552510000
C	-1.512075000	-0.974632000	-0.253293000
S	-2.730571000	0.258533000	0.047144000
C	-4.048021000	-0.867972000	-0.216766000
C	-3.533386000	-2.131944000	-0.532158000
H	-1.596238000	-3.101751000	-0.762801000

H	-4.161153000	-2.993075000	-0.721520000
C	-5.429963000	-0.466823000	-0.108291000
C	-6.461812000	-1.352413000	-0.495816000
C	-5.797323000	0.811267000	0.378602000
H	-6.224366000	-2.333284000	-0.888844000
H	-5.031040000	1.512218000	0.699265000
C	-7.791765000	-0.975035000	-0.399321000
C	-7.122648000	1.196453000	0.478902000
H	-8.574840000	-1.663616000	-0.705130000
C	-8.145748000	0.289550000	0.083961000
O	-7.539776000	2.396940000	0.940427000
H	-6.779480000	2.942680000	1.183418000
O	-9.411894000	0.721778000	0.206118000
H	-10.031016000	0.035801000	-0.082393000

A6+

C	-5.777999000	-0.058973000	0.015622000
C	-5.305430000	-1.369013000	0.302882000
C	-4.820930000	0.952024000	-0.272940000
H	-6.013559000	-2.147839000	0.557642000
H	-5.157558000	1.949397000	-0.527291000
C	-3.958479000	-1.642676000	0.307595000
C	-3.477236000	0.661661000	-0.278278000
H	-3.635992000	-2.643081000	0.571251000
H	-2.779403000	1.450477000	-0.540118000
C	-2.990096000	-0.641802000	0.014142000
N	-7.130770000	0.225408000	0.017382000
C	-8.101983000	-0.794372000	-0.239650000
C	-9.223093000	-0.908213000	0.595819000
C	-7.945508000	-1.653447000	-1.338631000
C	-10.174151000	-1.890548000	0.336280000
C	-8.905074000	-2.631414000	-1.587093000
C	-10.018464000	-2.754093000	-0.751868000
H	-9.334532000	-0.241173000	1.443597000
H	-7.092753000	-1.536308000	-1.998876000
H	-11.036010000	-1.985892000	0.988515000
H	-8.790188000	-3.288217000	-2.443159000
H	-10.765069000	-3.515759000	-0.951372000
C	-7.605967000	1.550350000	0.280063000
C	-7.117403000	2.265690000	1.384402000
C	-8.582386000	2.113500000	-0.554928000
C	-7.599641000	3.546766000	1.639750000
C	-9.054815000	3.395262000	-0.288748000
C	-8.565846000	4.114803000	0.805475000
H	-6.386197000	1.809580000	2.043286000
H	-8.952027000	1.553236000	-1.406775000
H	-7.230665000	4.095692000	2.499964000
H	-9.802418000	3.835604000	-0.940278000
H	-8.940733000	5.112252000	1.010203000
C	-0.971164000	-2.193422000	0.172940000
C	-1.588218000	-0.945879000	0.019030000
S	-0.363117000	0.299274000	-0.175227000
C	0.939118000	-0.861904000	-0.058114000
C	0.422939000	-2.146039000	0.129520000
H	-1.523496000	-3.117064000	0.292744000
H	1.049133000	-3.025697000	0.206333000
C	2.332748000	-0.458081000	-0.145521000
C	3.340731000	-1.342599000	0.242490000

C	2.697578000	0.841040000	-0.620864000
H	3.122207000	-2.329795000	0.631815000
H	1.924693000	1.532086000	-0.941701000
C	4.696218000	-0.968086000	0.166799000
C	4.012019000	1.222000000	-0.700809000
H	4.276268000	2.209118000	-1.067761000
C	5.047428000	0.329347000	-0.308830000
C	6.893436000	-1.530625000	0.495799000
C	7.391311000	-0.250722000	0.034003000
C	6.416751000	0.658292000	-0.365935000
H	6.700612000	1.636801000	-0.732961000
N	5.643010000	-1.869681000	0.561971000
Cl	8.032487000	-2.755639000	1.035751000
C	8.821608000	0.010415000	-0.010102000
H	9.469346000	-0.841683000	0.170679000
C	9.501562000	1.166586000	-0.232923000
C	8.901522000	2.440380000	-0.467326000
N	8.387808000	3.467105000	-0.662219000
C	11.002623000	1.084555000	-0.216359000
O	11.621928000	0.061276000	-0.029542000
O	11.568257000	2.284354000	-0.433564000
H	12.531871000	2.156299000	-0.407120000

A7+

C	-5.558845000	-0.053989000	0.016871000
C	-5.113129000	-1.368746000	0.322514000
C	-4.581168000	0.936137000	-0.272728000
H	-5.837667000	-2.131596000	0.579532000
H	-4.897077000	1.936662000	-0.540970000
C	-3.771049000	-1.667094000	0.342017000
C	-3.242571000	0.621134000	-0.262455000
H	-3.469024000	-2.669784000	0.621209000
H	-2.527947000	1.393620000	-0.527887000
C	-2.782709000	-0.687550000	0.046796000
N	-6.906993000	0.254701000	0.001610000
C	-7.892987000	-0.749914000	-0.257607000
C	-9.025689000	-0.836579000	0.565505000
C	-7.739059000	-1.622116000	-1.346624000
C	-9.990767000	-1.804577000	0.303815000
C	-8.712520000	-2.585633000	-1.597290000
C	-9.837630000	-2.681058000	-0.774285000
H	-9.135328000	-0.159783000	1.405764000
H	-6.876683000	-1.526246000	-1.997739000
H	-10.861726000	-1.878642000	0.946680000
H	-8.599142000	-3.252402000	-2.445838000
H	-10.595108000	-3.431450000	-0.975528000
C	-7.360785000	1.590112000	0.247090000
C	-6.869833000	2.307803000	1.348911000
C	-8.318888000	2.162761000	-0.602648000
C	-7.330987000	3.599910000	1.586927000
C	-8.770611000	3.455378000	-0.353574000
C	-8.278972000	4.176996000	0.738053000
H	-6.153101000	1.845363000	2.019193000
H	-8.690582000	1.600868000	-1.452532000
H	-6.960038000	4.150740000	2.445088000
H	-9.503927000	3.902555000	-1.016603000
H	-8.637524000	5.183082000	0.929323000
C	-0.794417000	-2.279001000	0.201930000

C	-1.385440000	-1.017746000	0.065533000
S	-0.136641000	0.208027000	-0.085861000
C	1.144095000	-0.979717000	0.019608000
C	0.601703000	-2.256374000	0.176297000
H	-1.366003000	-3.194460000	0.290227000
H	1.209039000	-3.150727000	0.235297000
C	2.543250000	-0.597816000	-0.049672000
C	3.537965000	-1.495007000	0.374761000
C	2.929419000	0.676568000	-0.544703000
H	3.267898000	-2.462272000	0.784821000
H	2.176070000	1.372411000	-0.897914000
C	4.886585000	-1.140013000	0.306560000
C	4.260044000	1.027346000	-0.610713000
H	4.550263000	1.999661000	-0.996445000
C	5.271454000	0.135831000	-0.189893000
C	7.254213000	-1.739353000	0.699320000
C	7.638811000	-0.399824000	0.175154000
C	6.657709000	0.469076000	-0.241818000
H	6.921104000	1.447743000	-0.626133000
N	5.881809000	-1.994832000	0.719878000
H	5.644101000	-2.911659000	1.079946000
C	9.067103000	-0.158900000	0.166505000
C	9.780882000	0.932667000	-0.223735000
C	9.201268000	2.132154000	-0.734733000
N	8.689881000	3.094017000	-1.147383000
C	11.275194000	0.859779000	-0.102942000
O	11.876469000	-0.103801000	0.315172000
O	11.862781000	1.997922000	-0.516723000
H	12.821774000	1.878003000	-0.410174000
O	8.040860000	-2.585755000	1.093790000
H	9.663298000	-0.990114000	0.535320000

A8+

C	6.298362000	0.173797000	0.009241000
C	5.465588000	1.310559000	0.180357000
C	5.674022000	-1.078379000	-0.230917000
H	5.912109000	2.264825000	0.390004000
H	6.281894000	-1.948888000	-0.394214000
C	4.112063000	1.193750000	0.126212000
C	4.319409000	-1.175053000	-0.298781000
H	3.517063000	2.073368000	0.294821000
H	3.885298000	-2.136915000	-0.514440000
C	3.477398000	-0.050099000	-0.118561000
N	7.647470000	0.279406000	0.073330000
C	8.307973000	1.533307000	-0.109621000
C	9.225184000	1.967021000	0.839194000
C	8.057665000	2.287576000	-1.250017000
C	9.879433000	3.170674000	0.650041000
C	8.718327000	3.490364000	-1.428850000
C	9.627024000	3.934103000	-0.480498000
H	9.416568000	1.368226000	1.713246000
H	7.365636000	1.926774000	-1.992411000
H	10.585431000	3.513318000	1.387355000
H	8.531862000	4.073197000	-2.314937000
H	10.142199000	4.868689000	-0.624617000
C	8.473895000	-0.857583000	0.330905000
C	8.232712000	-1.649500000	1.447567000
C	9.536569000	-1.136577000	-0.519166000

C	9.051521000	-2.735920000	1.701110000
C	10.348306000	-2.224788000	-0.255861000
C	10.107380000	-3.026043000	0.850846000
H	7.422928000	-1.405995000	2.114773000
H	9.717639000	-0.509479000	-1.375384000
H	8.871182000	-3.347039000	2.569213000
H	11.168191000	-2.448455000	-0.917087000
H	10.744800000	-3.870140000	1.052862000
C	1.125388000	0.873069000	-0.059750000
C	2.064887000	-0.156374000	-0.177726000
S	1.248627000	-1.669759000	-0.419217000
C	-0.317008000	-0.919122000	-0.363096000
C	-0.187669000	0.453644000	-0.161805000
H	1.395859000	1.901824000	0.091224000
H	-1.021818000	1.126840000	-0.095793000
C	-1.468527000	-1.731941000	-0.518053000
C	-3.808905000	-2.394652000	-0.682989000
C	-2.770656000	-1.361598000	-0.491665000
S	-3.477050000	0.202155000	-0.254863000
C	-5.116641000	-0.464882000	-0.400026000
O	-3.609576000	-3.567015000	-0.857910000
N	-5.066023000	-1.818988000	-0.646517000
C	-6.209143000	-2.698682000	-0.772169000
C	-6.857677000	-3.107398000	0.533404000
O	-7.866052000	-3.741524000	0.568240000
O	-6.177656000	-2.706476000	1.603372000
H	-6.648240000	-3.019025000	2.380404000
C	-8.394272000	1.581077000	-0.049702000
S	-7.913430000	-0.085070000	-0.355791000
C	-6.202595000	0.323660000	-0.279088000
C	-6.057887000	1.759770000	-0.019333000
S	-9.959153000	2.024286000	0.036587000
N	-7.291902000	2.372166000	0.082891000
O	-5.008871000	2.351485000	0.093816000
C	-7.368463000	3.809086000	0.358567000
H	-6.497823000	4.250672000	-0.109786000
H	-8.261076000	4.175644000	-0.131434000
C	-7.395268000	4.104281000	1.846399000
H	-6.494526000	3.738144000	2.328997000
H	-8.260787000	3.650242000	2.317220000
H	-7.450074000	5.177620000	2.001264000
H	-6.962532000	-2.275878000	-1.423834000
H	-5.847971000	-3.607238000	-1.241178000
H	-1.317660000	-2.788868000	-0.678841000

Cartesian coordinates of the oxidized dyes using CAM-B3LYP

A1+

C	2.398721000	-0.080352000	-0.024376000
C	1.772757000	-1.279134000	-0.460762000
C	1.573056000	1.001253000	0.384600000
H	2.382446000	-2.101625000	-0.811362000
H	2.028923000	1.909573000	0.756341000
C	0.409850000	-1.378038000	-0.492549000
C	0.211534000	0.879785000	0.361552000
H	-0.033857000	-2.291277000	-0.868438000
H	-0.388183000	1.711245000	0.715192000

C	-0.424333000	-0.307658000	-0.079912000
N	3.761159000	0.030841000	0.000861000
C	4.598971000	-1.124186000	0.084485000
C	5.688686000	-1.242052000	-0.779617000
C	4.341192000	-2.102072000	1.047525000
C	6.509165000	-2.355588000	-0.687813000
C	5.173237000	-3.208993000	1.131055000
C	6.253895000	-3.339034000	0.264294000
H	5.877672000	-0.473394000	-1.520173000
H	3.511983000	-1.980616000	1.735639000
H	7.350104000	-2.457894000	-1.364311000
H	4.983787000	-3.965583000	1.884104000
H	6.902419000	-4.205163000	0.334597000
C	4.401298000	1.307588000	-0.057969000
C	4.022901000	2.229826000	-1.035927000
C	5.422721000	1.603154000	0.846111000
C	4.663263000	3.459073000	-1.094313000
C	6.051164000	2.836917000	0.778804000
C	5.673604000	3.765216000	-0.188005000
H	3.252130000	1.973394000	-1.754269000
H	5.706772000	0.875834000	1.597956000
H	4.380606000	4.174416000	-1.858354000
H	6.837095000	3.076409000	1.486085000
H	6.172570000	4.726557000	-0.238634000
C	-2.604220000	-1.560417000	-0.426017000
C	-1.853473000	-0.430464000	-0.112481000
S	-2.906077000	0.899578000	0.261793000
C	-4.325847000	-0.063145000	-0.000742000
C	-3.984039000	-1.358915000	-0.363426000
H	-2.166162000	-2.515302000	-0.685007000
H	-4.712671000	-2.129491000	-0.572562000
C	-5.608516000	0.564739000	0.175608000
H	-5.615957000	1.611854000	0.469310000
C	-6.839450000	0.026659000	0.024775000
C	-7.072324000	-1.328661000	-0.355204000
N	-7.211806000	-2.434860000	-0.665250000
C	-8.011433000	0.923174000	0.276084000
O	-7.903520000	2.079672000	0.599988000
O	-9.169845000	0.288241000	0.098257000
H	-9.885286000	0.920587000	0.275285000

A2+

C	3.037023000	-0.129047000	-0.042578000
C	2.555544000	-1.420959000	-0.396273000
C	2.081832000	0.881997000	0.258561000
H	3.261735000	-2.197046000	-0.660262000
H	2.423385000	1.862835000	0.561759000
C	1.215523000	-1.672565000	-0.451813000
C	0.745110000	0.609383000	0.214191000
H	0.887010000	-2.656726000	-0.761697000
H	0.047597000	1.394600000	0.484522000
C	0.252151000	-0.673265000	-0.145337000
N	4.372862000	0.132328000	0.006716000
C	5.336751000	-0.920018000	0.142673000
C	6.416203000	-0.976208000	-0.737380000
C	5.207533000	-1.850882000	1.173176000
C	7.359410000	-1.982879000	-0.591999000
C	6.158469000	-2.853083000	1.308624000

C	7.232245000	-2.921998000	0.427343000
H	6.507370000	-0.240320000	-1.528270000
H	4.379118000	-1.777053000	1.869313000
H	8.196299000	-2.035207000	-1.279320000
H	6.065781000	-3.574090000	2.113122000
H	7.974767000	-3.704337000	0.538495000
C	4.876909000	1.471642000	-0.076624000
C	4.477818000	2.299683000	-1.125654000
C	5.793781000	1.917346000	0.873914000
C	4.989291000	3.587475000	-1.209092000
C	6.297358000	3.206385000	0.779795000
C	5.896152000	4.042757000	-0.257947000
H	3.787616000	1.929332000	-1.875856000
H	6.100636000	1.258975000	1.678708000
H	4.687223000	4.231647000	-2.027292000
H	7.004561000	3.559935000	1.521690000
H	6.296085000	5.048146000	-0.328545000
C	-1.764704000	-2.177795000	-0.454838000
C	-1.144034000	-0.954314000	-0.200794000
S	-2.354483000	0.278805000	0.053134000
C	-3.651025000	-0.848244000	-0.165671000
C	-3.156725000	-2.115832000	-0.435570000
H	-1.219643000	-3.096147000	-0.629676000
H	-3.796251000	-2.976005000	-0.582104000
C	-5.046931000	-0.436244000	-0.069337000
C	-6.045537000	-1.203630000	-0.688086000
C	-5.416989000	0.717914000	0.634994000
C	-7.372548000	-0.827188000	-0.598785000
C	-6.745999000	1.094983000	0.722162000
C	-7.728436000	0.321759000	0.105851000
H	-5.777903000	-2.083495000	-1.261664000
H	-4.662696000	1.312966000	1.139426000
H	-8.154835000	-1.406391000	-1.075354000
H	-7.030144000	1.983391000	1.272384000
C	-9.173925000	0.677484000	0.167280000
O	-10.049756000	0.033215000	-0.356500000
O	-9.405811000	1.797433000	0.870806000
H	-10.364984000	1.944712000	0.854297000

A3+

C	-3.929527000	-0.242538000	0.060731000
C	-3.722630000	-1.594221000	0.457780000
C	-2.785922000	0.546045000	-0.251930000
H	-4.573747000	-2.204215000	0.729627000
H	-2.918827000	1.565977000	-0.587202000
C	-2.461581000	-2.108463000	0.541906000
C	-1.532643000	0.012144000	-0.176225000
H	-2.342738000	-3.129848000	0.881368000
H	-0.688524000	0.633744000	-0.453917000
C	-1.312548000	-1.333080000	0.226613000
N	-5.182953000	0.280634000	-0.018252000
C	-6.341454000	-0.558831000	-0.121432000
C	-7.406728000	-0.362587000	0.755305000
C	-6.408530000	-1.530748000	-1.119132000
C	-8.536782000	-1.158928000	0.640373000
C	-7.544986000	-2.321179000	-1.224268000
C	-8.607672000	-2.138439000	-0.345811000
H	-7.343090000	0.403395000	1.519898000

H	-5.584321000	-1.651854000	-1.813708000
H	-9.364796000	-1.014887000	1.325348000
H	-7.604132000	-3.073046000	-2.003295000
H	-9.495069000	-2.755349000	-0.433551000
C	-5.407105000	1.697298000	-0.002599000
C	-4.867789000	2.474869000	1.021619000
C	-6.197707000	2.274204000	-0.994703000
C	-5.109488000	3.841867000	1.038021000
C	-6.431850000	3.641205000	-0.967552000
C	-5.888422000	4.426311000	0.045049000
H	-4.278956000	2.007974000	1.803710000
H	-6.617361000	1.654822000	-1.779310000
H	-4.697374000	4.448919000	1.836328000
H	-7.039638000	4.095397000	-1.742050000
H	-6.077690000	5.493819000	0.063272000
C	0.347476000	-3.204794000	0.623947000
C	-0.001612000	-1.884957000	0.312779000
S	1.420804000	-0.918748000	0.019738000
C	2.467491000	-2.275631000	0.306689000
C	1.715144000	-3.414916000	0.617852000
H	-0.371089000	-3.984613000	0.838064000
H	2.182835000	-4.368760000	0.829390000
C	3.896752000	-2.341472000	0.262787000
H	4.259051000	-3.340282000	0.496053000
C	7.030669000	-0.159009000	-0.421942000
S	6.568490000	-1.808870000	0.014405000
C	4.860301000	-1.424593000	-0.007668000
C	4.672235000	-0.001179000	-0.354490000
O	3.610070000	0.581860000	-0.441397000
S	8.573316000	0.323209000	-0.590816000
N	5.897768000	0.607155000	-0.587702000
C	5.952822000	2.024409000	-0.886700000
C	6.176390000	2.911166000	0.325167000
O	6.341001000	4.097033000	0.235750000
O	6.142249000	2.234656000	1.481869000
H	6.303405000	2.880457000	2.189160000
H	4.998834000	2.305040000	-1.335304000
H	6.755402000	2.217221000	-1.598213000

A4+

C	3.704080000	-0.236419000	-0.034567000
C	3.249037000	-1.474218000	-0.512098000
C	2.784589000	0.699037000	0.460655000
H	3.951889000	-2.185152000	-0.929533000
H	3.134679000	1.643707000	0.858968000
C	1.898911000	-1.761205000	-0.498834000
C	1.437913000	0.392161000	0.483566000
H	1.558391000	-2.700797000	-0.917329000
H	0.745995000	1.111403000	0.908052000
C	0.967699000	-0.839293000	0.004373000
N	5.080607000	0.067035000	-0.057074000
C	6.027771000	-0.930685000	0.237260000
C	7.233798000	-0.978299000	-0.483879000
C	5.767129000	-1.869786000	1.250517000
C	8.162099000	-1.960023000	-0.190186000
C	6.711441000	-2.837424000	1.537346000
C	7.907245000	-2.887825000	0.819409000
H	7.412150000	-0.272570000	-1.286379000

H	4.851624000	-1.804904000	1.826462000
H	9.084637000	-2.012102000	-0.756812000
H	6.525784000	-3.549173000	2.333503000
H	8.641854000	-3.651958000	1.048103000
C	5.509885000	1.368313000	-0.380436000
C	4.849897000	2.094748000	-1.386354000
C	6.602982000	1.929228000	0.302181000
C	5.291370000	3.365311000	-1.705383000
C	7.023705000	3.205862000	-0.023024000
C	6.374421000	3.924688000	-1.026197000
H	4.031111000	1.642237000	-1.933168000
H	7.085152000	1.375040000	1.098689000
H	4.801838000	3.920248000	-2.497440000
H	7.854900000	3.649045000	0.513240000
H	6.713587000	4.922745000	-1.280570000
C	-1.019101000	-2.432333000	0.033693000
C	-0.459832000	-1.176708000	0.014849000
S	-1.675954000	0.056776000	-0.036841000
C	-2.945736000	-1.134525000	-0.005637000
C	-2.426706000	-2.410362000	0.010519000
H	-0.440911000	-3.345245000	0.090521000
H	-3.042813000	-3.301307000	0.036750000
C	-8.055318000	-1.003774000	-1.216657000
C	-6.750617000	-0.856277000	-0.751792000
C	-6.425476000	0.111686000	0.199390000
C	-7.394675000	0.977218000	0.706598000
C	-8.688079000	0.829587000	0.240562000
C	-9.016919000	-0.150402000	-0.706868000
C	-4.358370000	-0.839921000	-0.127764000
N	-5.064981000	0.066789000	0.544800000
H	-8.307514000	-1.756579000	-1.954354000
H	-7.154788000	1.747204000	1.430154000
H	-9.463109000	1.488348000	0.614754000
H	-10.041411000	-0.237469000	-1.049769000
S	-5.323088000	-1.737310000	-1.224602000
C	-4.532326000	0.942639000	1.582310000
C	-4.163459000	2.294052000	0.985058000
O	-3.734126000	2.416962000	-0.132309000
O	-4.352409000	3.270020000	1.863608000
H	-4.071688000	4.112691000	1.466091000
H	-3.636987000	0.488677000	2.010495000
H	-5.270956000	1.041497000	2.376520000

A5+

C	2.670583000	-0.152514000	-0.047245000
C	2.187846000	-1.453525000	-0.359726000
C	1.713476000	0.867303000	0.212223000
H	2.893829000	-2.241596000	-0.585236000
H	2.053080000	1.859484000	0.477771000
C	0.847651000	-1.706187000	-0.414845000
C	0.376475000	0.595437000	0.166519000
H	0.522465000	-2.702705000	-0.687365000
H	-0.320452000	1.393229000	0.400412000
C	-0.117961000	-0.697227000	-0.151374000
N	4.006283000	0.108495000	0.003003000
C	4.973540000	-0.944074000	-0.132617000
C	6.018073000	-1.030481000	-0.784568000
C	4.885005000	-1.843186000	1.193909000

C	6.968471000	-2.032027000	-0.643634000
C	5.839150000	-2.843859000	1.323354000
C	6.880070000	-2.940514000	0.406376000
H	6.080350000	-0.317202000	-1.598818000
H	4.080714000	-1.749459000	1.915747000
H	7.780153000	-2.103959000	-1.359050000
H	5.774779000	-3.541585000	2.151008000
H	7.626308000	-3.719972000	0.513225000
C	4.514287000	1.448676000	-0.073098000
C	4.167618000	2.264018000	-1.149111000
C	5.385613000	1.907192000	0.911963000
C	4.683928000	3.550889000	-1.225743000
C	5.899069000	3.193528000	0.823490000
C	5.548295000	4.017414000	-0.241424000
H	3.508379000	1.885723000	-1.923047000
H	5.655170000	1.257669000	1.737246000
H	4.419284000	4.185184000	-2.064567000
H	6.574302000	3.554146000	1.591503000
H	5.953864000	5.020933000	-0.307072000
C	-2.133349000	-2.209647000	-0.448171000
C	-1.508751000	-0.978604000	-0.207047000
S	-2.723475000	0.255384000	0.028713000
C	-4.026715000	-0.875542000	-0.181896000
C	-3.517044000	-2.151488000	-0.434210000
H	-1.584884000	-3.127141000	-0.615133000
H	-4.146989000	-3.018024000	-0.581652000
C	-5.407529000	-0.472338000	-0.095792000
C	-6.428376000	-1.358355000	-0.472961000
C	-5.772259000	0.812977000	0.359417000
H	-6.189564000	-2.346627000	-0.844790000
H	-5.007675000	1.517460000	0.674541000
C	-7.755561000	-0.975787000	-0.398251000
C	-7.091089000	1.200374000	0.438053000
H	-8.537265000	-1.667246000	-0.697988000
C	-8.106961000	0.292533000	0.052902000
O	-7.509602000	2.406707000	0.870049000
H	-6.755330000	2.957817000	1.111387000
O	-9.368082000	0.731131000	0.153306000
H	-9.988781000	0.045641000	-0.125755000

A6+

C	-5.739536000	-0.055543000	0.013715000
C	-5.272418000	-1.383268000	0.225663000
C	-4.775006000	0.962726000	-0.227817000
H	-5.984353000	-2.168584000	0.442591000
H	-5.106615000	1.973594000	-0.424713000
C	-3.936744000	-1.662280000	0.205591000
C	-3.443479000	0.664134000	-0.259434000
H	-3.617711000	-2.676880000	0.408929000
H	-2.740242000	1.459541000	-0.480757000
C	-2.964678000	-0.655032000	-0.041070000
N	-7.070313000	0.232597000	0.041288000
C	-8.060985000	-0.786112000	-0.148627000
C	-9.103907000	-0.904090000	0.768494000
C	-7.994413000	-1.620452000	-1.264220000
C	-10.073278000	-1.876874000	0.573245000
C	-8.971058000	-2.589584000	-1.448873000
C	-10.008451000	-2.720614000	-0.531766000

H	-9.146636000	-0.242747000	1.626480000
H	-7.194387000	-1.497047000	-1.986088000
H	-10.881754000	-1.977653000	1.288609000
H	-8.927055000	-3.235179000	-2.318888000
H	-10.771248000	-3.476611000	-0.681279000
C	-7.543033000	1.567707000	0.263011000
C	-7.090384000	2.290890000	1.366312000
C	-8.483066000	2.112898000	-0.609874000
C	-7.571945000	3.574771000	1.582827000
C	-8.956015000	3.396998000	-0.383139000
C	-8.501689000	4.129493000	0.709717000
H	-6.381886000	1.842596000	2.054335000
H	-8.831515000	1.534987000	-1.458373000
H	-7.228148000	4.137482000	2.443525000
H	-9.681060000	3.828167000	-1.064269000
H	-8.877872000	5.131376000	0.884215000
C	-0.968929000	-2.216841000	0.045474000
C	-1.573298000	-0.963914000	-0.063400000
S	-0.348268000	0.268086000	-0.235958000
C	0.932728000	-0.895873000	-0.171313000
C	0.422159000	-2.176557000	-0.015945000
H	-1.526173000	-3.138891000	0.146880000
H	1.048524000	-3.057747000	0.023248000
C	2.332142000	-0.497215000	-0.263514000
C	3.320740000	-1.347913000	0.195895000
C	2.698560000	0.762927000	-0.816941000
H	3.094055000	-2.304549000	0.650470000
H	1.929738000	1.427498000	-1.196326000
C	4.677059000	-0.978772000	0.116256000
C	4.008936000	1.136223000	-0.900917000
H	4.281322000	2.095960000	-1.327421000
C	5.031837000	0.273737000	-0.434727000
C	6.857949000	-1.516500000	0.517057000
C	7.355731000	-0.275492000	-0.016878000
C	6.402965000	0.599011000	-0.492273000
H	6.695174000	1.548390000	-0.923234000
N	5.612702000	-1.850060000	0.585319000
Cl	7.991825000	-2.680276000	1.153442000
C	8.790660000	-0.014927000	-0.069188000
H	9.446548000	-0.878279000	-0.019376000
C	9.438520000	1.162542000	-0.156661000
C	8.797089000	2.440842000	-0.187139000
N	8.246911000	3.458097000	-0.223762000
C	10.934145000	1.117635000	-0.206792000
O	11.574991000	0.096911000	-0.191616000
O	11.467710000	2.340860000	-0.268847000
H	12.432423000	2.235216000	-0.294439000

A7+

C	-5.529852000	-0.053305000	0.006857000
C	-5.087391000	-1.391857000	0.201081000
C	-4.546247000	0.953602000	-0.201210000
H	-5.814813000	-2.169275000	0.393827000
H	-4.858885000	1.972738000	-0.386340000
C	-3.755720000	-1.691736000	0.196154000
C	-3.218881000	0.634386000	-0.217394000
H	-3.455348000	-2.714371000	0.387510000
H	-2.499821000	1.421810000	-0.415093000

C	-2.764963000	-0.695708000	-0.016223000
N	-6.856811000	0.255916000	0.019953000
C	-7.859738000	-0.741566000	-0.210346000
C	-8.924239000	-0.858165000	0.682188000
C	-7.782864000	-1.556779000	-1.339587000
C	-9.904913000	-1.810796000	0.448684000
C	-8.771447000	-2.505367000	-1.562745000
C	-9.830289000	-2.635326000	-0.670219000
H	-8.974367000	-0.212045000	1.551275000
H	-6.965962000	-1.433490000	-2.042268000
H	-10.730057000	-1.910975000	1.144819000
H	-8.719843000	-3.135469000	-2.443615000
H	-10.602186000	-3.375351000	-0.849873000
C	-7.310897000	1.592612000	0.266421000
C	-6.856120000	2.285480000	1.388430000
C	-8.235004000	2.170755000	-0.602670000
C	-7.319287000	3.571950000	1.627744000
C	-8.689165000	3.457265000	-0.353127000
C	-8.232575000	4.159467000	0.758609000
H	-6.161181000	1.811563000	2.073040000
H	-8.584785000	1.616565000	-1.466272000
H	-6.974352000	4.111075000	2.502938000
H	-9.401105000	3.914289000	-1.031189000
H	-8.594263000	5.163433000	0.950846000
C	-0.794531000	-2.290756000	0.046615000
C	-1.376715000	-1.025993000	-0.022309000
S	-0.131178000	0.193046000	-0.117475000
C	1.131137000	-0.992206000	-0.079265000
C	0.599533000	-2.269050000	0.014249000
H	-1.367610000	-3.207500000	0.094286000
H	1.211098000	-3.161526000	0.023079000
C	2.536292000	-0.606830000	-0.134857000
C	3.509158000	-1.475500000	0.358055000
C	2.924413000	0.633348000	-0.681417000
H	3.226556000	-2.419251000	0.811395000
H	2.178779000	1.305687000	-1.090416000
C	4.856321000	-1.121100000	0.306053000
C	4.254219000	0.981501000	-0.729224000
H	4.554854000	1.932729000	-1.155833000
C	5.245831000	0.118100000	-0.239517000
C	7.200478000	-1.694596000	0.790132000
C	7.595992000	-0.386667000	0.211798000
C	6.639103000	0.451909000	-0.270619000
H	6.910517000	1.410202000	-0.696662000
N	5.837436000	-1.952923000	0.788085000
H	5.591983000	-2.849599000	1.187720000
C	9.029061000	-0.146133000	0.230999000
C	9.744199000	0.918075000	-0.187990000
C	9.172818000	2.091468000	-0.770820000
N	8.663231000	3.020373000	-1.237376000
C	11.229043000	0.860019000	-0.027639000
O	11.821495000	-0.074818000	0.449199000
O	11.821878000	1.972510000	-0.477628000
H	12.776657000	1.863039000	-0.341724000
O	7.978198000	-2.511499000	1.244353000
H	9.612875000	-0.959153000	0.654781000

A8+

C	6.312032000	0.173985000	0.011089000
C	5.477271000	1.314179000	0.182580000
C	5.686670000	-1.082511000	-0.226995000
H	5.927713000	2.275301000	0.391665000
H	6.299652000	-1.958808000	-0.390474000
C	4.118923000	1.196588000	0.129905000
C	4.327302000	-1.180015000	-0.293172000
H	3.518340000	2.081737000	0.298534000
H	3.888951000	-2.148747000	-0.507860000
C	3.483302000	-0.051429000	-0.113262000
N	7.667152000	0.280888000	0.073034000
C	8.329141000	1.541164000	-0.104872000
C	9.255085000	1.967562000	0.844911000
C	8.071062000	2.305995000	-1.241654000
C	9.911347000	3.175981000	0.660075000
C	8.733270000	3.513866000	-1.415298000
C	9.651208000	3.950783000	-0.466273000
H	9.452018000	1.356798000	1.718763000
H	7.369204000	1.947969000	-1.987090000
H	10.627567000	3.514510000	1.400385000
H	8.539910000	4.108197000	-2.301380000
H	10.169531000	4.892716000	-0.607243000
C	8.498932000	-0.861197000	0.322237000
C	8.258127000	-1.664830000	1.435856000
C	9.565463000	-1.130564000	-0.532923000
C	9.082115000	-2.755061000	1.680748000
C	10.382736000	-2.222219000	-0.277349000
C	10.142421000	-3.035972000	0.825773000
H	7.441615000	-1.426418000	2.108838000
H	9.745447000	-0.490711000	-1.389441000
H	8.901500000	-3.378682000	2.549201000
H	11.209478000	-2.439380000	-0.944399000
H	10.786242000	-3.886073000	1.022196000
C	1.122206000	0.872256000	-0.053355000
C	2.066080000	-0.158043000	-0.171729000
S	1.251667000	-1.678084000	-0.414057000
C	-0.317210000	-0.930133000	-0.357860000
C	-0.193750000	0.447579000	-0.155927000
H	1.393016000	1.908555000	0.098882000
H	-1.037186000	1.121041000	-0.089847000
C	-1.471469000	-1.748573000	-0.513731000
C	-3.816669000	-2.415509000	-0.679904000
C	-2.775901000	-1.376297000	-0.487264000
S	-3.482422000	0.192378000	-0.250159000
C	-5.127576000	-0.476914000	-0.399014000
O	-3.614814000	-3.595978000	-0.855739000
N	-5.079788000	-1.836689000	-0.643602000
C	-6.228276000	-2.717065000	-0.761827000
C	-6.900647000	-3.083515000	0.549733000
O	-7.926784000	-3.704387000	0.595154000
O	-6.216107000	-2.660925000	1.621716000
H	-6.713038000	-2.951775000	2.404213000
C	-8.411551000	1.586194000	-0.064452000
S	-7.930464000	-0.089502000	-0.365722000
C	-6.215987000	0.316569000	-0.282136000
C	-6.063188000	1.755973000	-0.023445000
S	-9.976493000	2.039964000	0.014779000
N	-7.300549000	2.377670000	0.072148000

O	-5.003323000	2.346178000	0.094330000
C	-7.372865000	3.817471000	0.348904000
H	-6.485935000	4.256157000	-0.109290000
H	-8.262253000	4.192337000	-0.157628000
C	-7.419871000	4.110707000	1.840721000
H	-6.523124000	3.734985000	2.338611000
H	-8.300665000	3.658168000	2.300419000
H	-7.470493000	5.190346000	1.999699000
H	-6.974625000	-2.309338000	-1.443369000
H	-5.855934000	-3.645817000	-1.200213000
H	-1.321408000	-2.813367000	-0.675909000

Cartesian coordinates of the oxidized dyes using
BHandHLYP

A1+

C	2.393908000	-0.078861000	-0.025987000
C	1.767224000	-1.275377000	-0.456453000
C	1.570450000	1.002498000	0.376497000
H	2.370930000	-2.095187000	-0.799963000
H	2.023046000	1.905967000	0.741695000
C	0.409297000	-1.372146000	-0.489065000
C	0.213761000	0.883131000	0.353470000
H	-0.030349000	-2.280802000	-0.858941000
H	-0.379573000	1.711790000	0.701111000
C	-0.423045000	-0.302003000	-0.082415000
N	3.749307000	0.029981000	0.000213000
C	4.583378000	-1.121679000	0.085464000
C	5.661877000	-1.248562000	-0.784284000
C	4.334609000	-2.088055000	1.056056000
C	6.479088000	-2.358918000	-0.690978000
C	5.163493000	-3.191611000	1.142046000
C	6.232515000	-3.330576000	0.269181000
H	5.845225000	-0.491916000	-1.527641000
H	3.517244000	-1.961689000	1.745675000
H	7.307722000	-2.467517000	-1.369730000
H	4.981514000	-3.935783000	1.898580000
H	6.876223000	-4.190834000	0.340707000
C	4.389906000	1.301072000	-0.058603000
C	4.026530000	2.215228000	-1.043512000
C	5.397839000	1.600305000	0.852575000
C	4.667681000	3.439063000	-1.102339000
C	6.026940000	2.828808000	0.785740000
C	5.664183000	3.748691000	-0.188547000
H	3.268793000	1.958427000	-1.764293000
H	5.671040000	0.882619000	1.606875000
H	4.397595000	4.144777000	-1.869312000
H	6.799051000	3.069911000	1.496263000
H	6.161970000	4.702207000	-0.238930000
C	-2.595155000	-1.549348000	-0.431667000
C	-1.845764000	-0.421906000	-0.114819000
S	-2.898423000	0.901990000	0.262865000
C	-4.316039000	-0.060930000	-0.002210000
C	-3.969654000	-1.351622000	-0.368749000
H	-2.159421000	-2.496187000	-0.692830000
H	-4.689759000	-2.119285000	-0.579575000
C	-5.593437000	0.559980000	0.175901000
H	-5.598780000	1.598347000	0.471064000

C	-6.823711000	0.024010000	0.025091000
C	-7.056572000	-1.326253000	-0.358208000
N	-7.199416000	-2.423136000	-0.669530000
C	-7.991076000	0.916415000	0.280044000
O	-7.880558000	2.063273000	0.605647000
O	-9.143157000	0.290332000	0.103520000
H	-9.856556000	0.908429000	0.279907000

A2+

C	3.031358000	-0.127302000	-0.042744000
C	2.548162000	-1.412796000	-0.401030000
C	2.080087000	0.880632000	0.261961000
H	3.247200000	-2.184253000	-0.666500000
H	2.420002000	1.852909000	0.567446000
C	1.212359000	-1.660811000	-0.457537000
C	0.747378000	0.611659000	0.216614000
H	0.886070000	-2.636483000	-0.770166000
H	0.057366000	1.392236000	0.489148000
C	0.252745000	-0.664470000	-0.147497000
N	4.361845000	0.130503000	0.007598000
C	5.319903000	-0.919591000	0.143908000
C	6.392648000	-0.983521000	-0.737102000
C	5.193462000	-1.843068000	1.175627000
C	7.330533000	-1.989025000	-0.591721000
C	6.139124000	-2.843963000	1.311939000
C	7.205680000	-2.920092000	0.429375000
H	6.483228000	-0.257026000	-1.526451000
H	4.373959000	-1.765299000	1.870231000
H	8.158425000	-2.046677000	-1.277770000
H	6.048484000	-3.555619000	2.114975000
H	7.941433000	-3.698511000	0.540413000
C	4.866239000	1.463806000	-0.075249000
C	4.477804000	2.287447000	-1.126064000
C	5.773260000	1.910958000	0.877839000
C	4.989568000	3.570310000	-1.209470000
C	6.276985000	3.195199000	0.784602000
C	5.886327000	4.026392000	-0.255523000
H	3.797607000	1.919174000	-1.875609000
H	6.072012000	1.259972000	1.681584000
H	4.696855000	4.207658000	-2.026559000
H	6.973404000	3.547927000	1.526207000
H	6.285040000	5.024256000	-0.325424000
C	-1.758513000	-2.160778000	-0.460624000
C	-1.139200000	-0.941535000	-0.203761000
S	-2.347469000	0.286440000	0.052132000
C	-3.643007000	-0.839308000	-0.169666000
C	-3.146251000	-2.100587000	-0.441801000
H	-1.217546000	-3.072536000	-0.636577000
H	-3.777772000	-2.957013000	-0.590486000
C	-5.034332000	-0.432547000	-0.072224000
C	-6.032738000	-1.211828000	-0.668697000
C	-5.403808000	0.729800000	0.611347000
C	-7.355794000	-0.839794000	-0.577637000
C	-6.729276000	1.102100000	0.700494000
C	-7.710864000	0.317268000	0.106880000
H	-5.769410000	-2.094991000	-1.224448000
H	-4.654815000	1.333714000	1.096319000
H	-8.131396000	-1.427895000	-1.036492000

H	-7.008890000	1.993352000	1.233267000
C	-9.151795000	0.669528000	0.172528000
O	-10.021923000	0.016943000	-0.330200000
O	-9.382227000	1.792918000	0.852059000
H	-10.329750000	1.945171000	0.846106000

O	6.269757000	4.088679000	0.226380000
O	6.106914000	2.244650000	1.474799000
H	6.236763000	2.882998000	2.180516000
H	5.033422000	2.292953000	-1.369642000
H	6.785202000	2.203898000	-1.563840000

A3+

C	-3.922549000	-0.240930000	0.060311000
C	-3.711154000	-1.587624000	0.458352000
C	-2.783991000	0.547912000	-0.253173000
H	-4.553710000	-2.196258000	0.729569000
H	-2.918203000	1.559754000	-0.587826000
C	-2.452998000	-2.095897000	0.542688000
C	-1.533483000	0.019885000	-0.177338000
H	-2.333525000	-3.109241000	0.881838000
H	-0.698193000	0.640188000	-0.454969000
C	-1.308858000	-1.320195000	0.226682000
N	-5.171646000	0.275893000	-0.018850000
C	-6.323042000	-0.564199000	-0.122779000
C	-7.381882000	-0.381163000	0.757751000
C	-6.391501000	-1.525232000	-1.124856000
C	-8.505382000	-1.178996000	0.642454000
C	-7.521460000	-2.316999000	-1.231268000
C	-8.577109000	-2.147220000	-0.348684000
H	-7.319315000	0.373307000	1.523243000
H	-5.576298000	-1.637070000	-1.819949000
H	-9.324634000	-1.045569000	1.328328000
H	-7.580996000	-3.056918000	-2.011352000
H	-9.456230000	-2.762864000	-0.436643000
C	-5.399600000	1.686496000	-0.002722000
C	-4.872674000	2.462213000	1.023491000
C	-6.181288000	2.261938000	-0.996739000
C	-5.117536000	3.824106000	1.040664000
C	-6.418428000	3.623889000	-0.969639000
C	-5.887342000	4.406475000	0.045509000
H	-4.292496000	1.999888000	1.804401000
H	-6.590798000	1.647996000	-1.780610000
H	-4.716623000	4.426546000	1.838063000
H	-7.016606000	4.074601000	-1.743229000
H	-6.078407000	5.466069000	0.063830000
C	0.348962000	-3.181355000	0.626240000
C	-0.001026000	-1.865088000	0.312990000
S	1.416984000	-0.901764000	0.019032000
C	2.464403000	-2.256660000	0.307626000
C	1.711618000	-3.391040000	0.620399000
H	-0.363929000	-3.955885000	0.840673000
H	2.173962000	-4.339046000	0.832506000
C	3.885863000	-2.325409000	0.263728000
H	4.243899000	-3.317723000	0.496284000
C	7.022084000	-0.166349000	-0.417316000
S	6.553473000	-1.806343000	0.016395000
C	4.852165000	-1.413782000	-0.007147000
C	4.675832000	0.005854000	-0.353348000
O	3.625950000	0.592200000	-0.440758000
S	8.567281000	0.300348000	-0.583682000
N	5.900538000	0.602847000	-0.583932000
C	5.962334000	2.015187000	-0.886804000
C	6.137995000	2.907703000	0.322428000

A4+

C	3.695609000	-0.235659000	-0.039697000
C	3.240917000	-1.469536000	-0.516571000
C	2.777820000	0.697648000	0.451689000
H	3.938426000	-2.176954000	-0.929218000
H	3.124383000	1.635917000	0.847570000
C	1.895128000	-1.754329000	-0.506967000
C	1.435310000	0.392981000	0.472429000
H	1.558551000	-2.686827000	-0.924841000
H	0.749347000	1.108265000	0.893849000
C	0.965417000	-0.834574000	-0.006508000
N	5.066787000	0.065050000	-0.058702000
C	6.007949000	-0.928555000	0.243647000
C	7.211024000	-0.985787000	-0.473550000
C	5.745545000	-1.855485000	1.261886000
C	8.133322000	-1.964591000	-0.172175000
C	6.684232000	-2.819474000	1.557797000
C	7.876804000	-2.879919000	0.842973000
H	7.392108000	-0.291775000	-1.275411000
H	4.836001000	-1.785079000	1.832378000
H	9.049356000	-2.023901000	-0.734295000
H	6.497608000	-3.518090000	2.355171000
H	8.604224000	-3.638476000	1.077352000
C	5.496725000	1.359383000	-0.385761000
C	4.846342000	2.077586000	-1.398114000
C	6.581243000	1.923907000	0.299045000
C	5.288358000	3.342005000	-1.721381000
C	7.001939000	3.194925000	-0.029130000
C	6.362359000	3.905224000	-1.039168000
H	4.036820000	1.625667000	-1.944237000
H	7.056071000	1.378939000	1.095997000
H	4.808224000	3.887365000	-2.515598000
H	7.822656000	3.638917000	0.507465000
H	6.700548000	4.894914000	-1.295372000
C	-1.016002000	-2.419908000	0.010146000
C	-0.457284000	-1.169231000	0.001680000
S	-1.672229000	0.060670000	-0.038330000
C	-2.939121000	-1.128133000	-0.015610000
C	-2.419924000	-2.398174000	-0.011770000
H	-0.443128000	-3.327847000	0.058770000
H	-3.029812000	-3.284613000	0.007529000
C	-8.036677000	-1.000813000	-1.205675000
C	-6.735041000	-0.853046000	-0.747125000
C	-6.406026000	0.112169000	0.198682000
C	-7.371562000	0.973272000	0.708005000
C	-8.662863000	0.825894000	0.248570000
C	-8.994257000	-0.150428000	-0.694690000
C	-4.348077000	-0.835208000	-0.130581000
N	-5.049249000	0.068532000	0.537897000
H	-8.289500000	-1.749018000	-1.936819000
H	-7.133571000	1.736866000	1.427596000
H	-9.431103000	1.479664000	0.623821000

H	-10.012855000	-0.237151000	-1.031482000
S	-5.312332000	-1.731632000	-1.221881000
C	-4.518668000	0.938729000	1.574590000
C	-4.155404000	2.292561000	0.993396000
O	-3.801806000	2.439144000	-0.137518000
O	-4.254194000	3.237249000	1.906650000
H	-3.986341000	4.081130000	1.529985000
H	-3.628987000	0.489456000	2.000503000
H	-5.251646000	1.031199000	2.364874000

A5+

C	2.665925000	-0.150528000	-0.047087000
C	2.182166000	-1.444871000	-0.366386000
C	1.712422000	0.865211000	0.218302000
H	2.881354000	-2.227596000	-0.595406000
H	2.049963000	1.848670000	0.488079000
C	0.846247000	-1.694632000	-0.422333000
C	0.379539000	0.596361000	0.171466000
H	0.523549000	-2.682513000	-0.699126000
H	-0.310259000	1.388873000	0.409139000
C	-0.115737000	-0.689507000	-0.153219000
N	3.996591000	0.107663000	0.003925000
C	4.957970000	-0.942374000	0.134801000
C	5.995026000	-1.038253000	-0.783469000
C	4.872659000	-1.832795000	1.198049000
C	6.939873000	-2.038771000	-0.641708000
C	5.821257000	-2.832378000	1.329140000
C	6.854259000	-2.937767000	0.410900000
H	6.056345000	-0.335629000	-1.597076000
H	4.077883000	-1.733823000	1.918517000
H	7.742082000	-2.117223000	-1.355859000
H	5.759130000	-3.519769000	2.155889000
H	7.593543000	-3.713434000	0.518264000
C	4.503862000	1.441963000	-0.073249000
C	4.166750000	2.251452000	-1.151169000
C	5.364961000	1.904093000	0.913114000
C	4.682013000	3.533857000	-1.229293000
C	5.877281000	3.186025000	0.823964000
C	5.536060000	4.003143000	-0.243553000
H	3.517759000	1.873730000	-1.923591000
H	5.627235000	1.263326000	1.737746000
H	4.425660000	4.160158000	-2.067098000
H	6.541617000	3.547354000	1.590649000
H	5.939385000	4.999479000	-0.309703000
C	-2.125284000	-2.193413000	-0.457943000
C	-1.502718000	-0.967769000	-0.210013000
S	-2.715283000	0.259701000	0.032986000
C	-4.016361000	-0.868754000	-0.184652000
C	-3.504950000	-2.137160000	-0.443791000
H	-1.580961000	-3.103635000	-0.629976000
H	-4.127509000	-2.998800000	-0.597109000
C	-5.393364000	-0.470524000	-0.096669000
C	-6.411421000	-1.357525000	-0.464874000
C	-5.760148000	0.812125000	0.352140000
H	-6.175282000	-2.340842000	-0.829498000
H	-5.002119000	1.516016000	0.658012000
C	-7.734463000	-0.978094000	-0.386946000
C	-7.074534000	1.195731000	0.433546000

H	-8.509923000	-1.668362000	-0.678436000
C	-8.086760000	0.287266000	0.057931000
O	-7.488019000	2.398225000	0.859213000
H	-6.746475000	2.951068000	1.093763000
O	-9.342995000	0.717978000	0.159014000
H	-9.961654000	0.041795000	-0.110241000

A6+

C	-5.727626000	-0.054273000	0.014187000
C	-5.256478000	-1.374238000	0.238198000
C	-4.768528000	0.961893000	-0.234098000
H	-5.960143000	-2.155509000	0.458765000
H	-5.100182000	1.962933000	-0.439163000
C	-3.924416000	-1.647329000	0.223496000
C	-3.440374000	0.669138000	-0.260543000
H	-3.606039000	-2.652273000	0.435310000
H	-2.745823000	1.460544000	-0.486400000
C	-2.957552000	-0.642056000	-0.029725000
N	-7.053626000	0.227945000	0.036577000
C	-8.036159000	-0.791630000	-0.150033000
C	-9.072251000	-0.916626000	0.767388000
C	-7.970201000	-1.622275000	-1.263030000
C	-10.034067000	-1.891237000	0.575376000
C	-8.939315000	-2.593047000	-1.445302000
C	-9.969416000	-2.730534000	-0.527554000
H	-9.116200000	-0.261473000	1.620569000
H	-7.179042000	-1.495776000	-1.982902000
H	-10.833566000	-1.996632000	1.288882000
H	-8.895503000	-3.232487000	-2.310593000
H	-10.723629000	-3.485007000	-0.674279000
C	-7.529896000	1.557281000	0.249765000
C	-7.091021000	2.282623000	1.351806000
C	-8.460051000	2.097677000	-0.629849000
C	-7.575825000	3.561714000	1.560723000
C	-8.936283000	3.377209000	-0.411471000
C	-8.495529000	4.111000000	0.680555000
H	-6.392563000	1.841639000	2.043030000
H	-8.797940000	1.521932000	-1.474498000
H	-7.243825000	4.122895000	2.417679000
H	-9.650567000	3.802352000	-1.095902000
H	-8.872965000	5.105511000	0.848103000
C	-0.964553000	-2.191638000	0.078695000
C	-1.569944000	-0.944544000	-0.046229000
S	-0.349148000	0.282894000	-0.231061000
C	0.933135000	-0.876999000	-0.149715000
C	0.421845000	-2.151235000	0.020085000
H	-1.516121000	-3.107179000	0.189935000
H	1.041623000	-3.027328000	0.072044000
C	2.326685000	-0.482111000	-0.244931000
C	3.315219000	-1.337563000	0.197424000
C	2.692015000	0.780734000	-0.784283000
H	3.090944000	-2.292408000	0.638336000
H	1.928452000	1.447631000	-1.148011000
C	4.666793000	-0.971033000	0.114090000
C	3.997781000	1.151209000	-0.871895000
H	4.266415000	2.108955000	-1.285945000
C	5.019223000	0.283948000	-0.423098000
C	6.840166000	-1.517198000	0.493672000

C	7.336486000	-0.274326000	-0.026147000
C	6.385514000	0.605750000	-0.484490000
H	6.675581000	1.552131000	-0.903888000
N	5.599929000	-1.844492000	0.564409000
Cl	7.967786000	-2.688955000	1.107184000
C	8.767436000	-0.018151000	-0.085126000
H	9.413973000	-0.879505000	-0.058533000
C	9.418705000	1.154002000	-0.154231000
C	8.783392000	2.432018000	-0.149337000
N	8.242397000	3.445375000	-0.156712000
C	10.908208000	1.103957000	-0.219664000
O	11.537901000	0.086306000	-0.234338000
O	11.446015000	2.315356000	-0.258237000
H	12.400213000	2.217203000	-0.295258000

A7+

C	-5.518235000	-0.051994000	0.007419000
C	-5.072207000	-1.383759000	0.210110000
C	-4.539790000	0.953275000	-0.205133000
H	-5.791514000	-2.157574000	0.405124000
H	-4.852218000	1.963331000	-0.395845000
C	-3.744192000	-1.678258000	0.209109000
C	-3.215829000	0.639410000	-0.217529000
H	-3.444676000	-2.691948000	0.406464000
H	-2.505259000	1.423302000	-0.418284000
C	-2.758386000	-0.683744000	-0.007704000
N	-6.840435000	0.251691000	0.016509000
C	-7.835451000	-0.745837000	-0.213805000
C	-8.894250000	-0.871297000	0.677681000
C	-7.758313000	-1.554706000	-1.342312000
C	-9.867498000	-1.825098000	0.444289000
C	-8.739563000	-2.504182000	-1.566243000
C	-9.792163000	-2.642551000	-0.674377000
H	-8.946258000	-0.233318000	1.543298000
H	-6.949552000	-1.426784000	-2.042025000
H	-10.684417000	-1.931439000	1.137608000
H	-8.687534000	-3.126080000	-2.443754000
H	-10.555573000	-3.380574000	-0.853563000
C	-7.297647000	1.582119000	0.258746000
C	-6.854946000	2.274275000	1.380754000
C	-8.213179000	2.157895000	-0.614220000
C	-7.321030000	3.555499000	1.616549000
C	-8.670168000	3.439412000	-0.368991000
C	-8.225522000	4.140032000	0.743182000
H	-6.169042000	1.805813000	2.066375000
H	-8.553595000	1.608051000	-1.474913000
H	-6.986690000	4.090918000	2.488910000
H	-9.372309000	3.892254000	-1.048166000
H	-8.588214000	5.136287000	0.931588000
C	-0.791216000	-2.268155000	0.069339000
C	-1.373809000	-1.008232000	-0.009550000
S	-0.132127000	0.207204000	-0.111252000
C	1.130857000	-0.975264000	-0.062283000
C	0.598391000	-2.246421000	0.039611000
H	-1.358844000	-3.179163000	0.122493000
H	1.203175000	-3.134444000	0.056532000
C	2.530550000	-0.593835000	-0.119299000
C	3.503393000	-1.468577000	0.355089000

C	2.917608000	0.650018000	-0.648982000
H	3.224265000	-2.411437000	0.793863000
H	2.177210000	1.325787000	-1.041282000
C	4.845385000	-1.117587000	0.300861000
C	4.243092000	0.994951000	-0.699537000
H	4.540191000	1.944971000	-1.111976000
C	5.232835000	0.125048000	-0.228624000
C	7.179963000	-1.699434000	0.762477000
C	7.576905000	-0.389372000	0.202063000
C	6.621184000	0.455055000	-0.262540000
H	6.890060000	1.411515000	-0.674127000
N	5.824296000	-1.953630000	0.764304000
H	5.579958000	-2.847396000	1.149424000
C	9.006180000	-0.152694000	0.216616000
C	9.722003000	0.911465000	-0.189365000
C	9.153563000	2.092362000	-0.751270000
N	8.651398000	3.024179000	-1.199194000
C	11.202038000	0.845627000	-0.037530000
O	11.786833000	-0.092898000	0.419697000
O	11.795772000	1.952628000	-0.469758000
H	12.741629000	1.847994000	-0.345385000
O	7.953347000	-2.518057000	1.198298000
H	9.585478000	-0.967065000	0.622817000

A8+

C	6.298362000	0.173797000	0.009241000
C	5.465588000	1.310559000	0.180357000
C	5.674022000	-1.078379000	-0.230917000
H	5.912109000	2.264825000	0.390004000
H	6.281894000	-1.948888000	-0.394214000
C	4.112063000	1.193750000	0.126212000
C	4.319409000	-1.175053000	-0.298781000
H	3.517063000	2.073368000	0.294821000
H	3.885298000	-2.136915000	-0.514440000
C	3.477398000	-0.050099000	-0.118561000
N	7.647470000	0.279406000	0.073330000
C	8.307973000	1.533307000	-0.109621000
C	9.225184000	1.967021000	0.839194000
C	8.057665000	2.287576000	-1.250017000
C	9.879433000	3.170674000	0.650041000
C	8.718327000	3.490364000	-1.428850000
C	9.627024000	3.934103000	-0.480498000
H	9.416568000	1.368226000	1.713246000
H	7.365636000	1.926774000	-1.992411000
H	10.585431000	3.513318000	1.387355000
H	8.531862000	4.073197000	-2.314937000
H	10.142199000	4.868689000	-0.624617000
C	8.473895000	-0.857583000	0.330905000
C	8.232712000	-1.649500000	1.447567000
C	9.536569000	-1.136577000	-0.519166000
C	9.051521000	-2.735920000	1.701110000
C	10.348306000	-2.224788000	-0.255861000
C	10.107380000	-3.026043000	0.850846000
H	7.422928000	-1.405995000	2.114773000
H	9.717639000	-0.509479000	-1.375384000
H	8.871182000	-3.347039000	2.569213000
H	11.168191000	-2.448455000	-0.917087000
H	10.744800000	-3.870140000	1.052862000

C	1.125388000	0.873069000	-0.059750000
C	2.064887000	-0.156374000	-0.177726000
S	1.248627000	-1.669759000	-0.419217000
C	-0.317008000	-0.919122000	-0.363096000
C	-0.187669000	0.453644000	-0.161805000
H	1.395859000	1.901824000	0.091224000
H	-1.021818000	1.126840000	-0.095793000
C	-1.468527000	-1.731941000	-0.518053000
C	-3.808905000	-2.394652000	-0.682989000
C	-2.770656000	-1.361598000	-0.491665000
S	-3.477050000	0.202155000	-0.254863000
C	-5.116641000	-0.464882000	-0.400026000
O	-3.609576000	-3.567015000	-0.857910000
N	-5.066023000	-1.818988000	-0.646517000
C	-6.209143000	-2.698682000	-0.772169000
C	-6.857677000	-3.107398000	0.533404000
O	-7.866052000	-3.741524000	0.568240000
O	-6.177656000	-2.706476000	1.603372000
H	-6.648240000	-3.019025000	2.380404000
C	-8.394272000	1.581077000	-0.049702000
S	-7.913430000	-0.085070000	-0.355791000
C	-6.202595000	0.323660000	-0.279088000
C	-6.057887000	1.759770000	-0.019333000
S	-9.959153000	2.024286000	0.036587000
N	-7.291902000	2.372166000	0.082891000
O	-5.008871000	2.351485000	0.093816000
C	-7.368463000	3.809086000	0.358567000
H	-6.497823000	4.250672000	-0.109786000
H	-8.261076000	4.175644000	-0.131434000
C	-7.395268000	4.104281000	1.846399000
H	-6.494526000	3.738144000	2.328997000
H	-8.260787000	3.650242000	2.317220000
H	-7.450074000	5.177620000	2.001264000
H	-6.962532000	-2.275878000	-1.423834000
H	-5.847971000	-3.607238000	-1.241178000
H	-1.317660000	-2.788868000	-0.678841000

Cartesian coordinates of the ground states of dye-(TiO₂)₁₅ systems using B3LYP

A1-(TiO₂)₁₅

Ti	1.925179000	-0.865052000	2.612795000
Ti	4.126925000	3.030284000	-1.727623000
Ti	6.188818000	1.125394000	-2.668559000
Ti	6.613970000	-1.435354000	1.488456000
Ti	3.080623000	-0.407608000	-3.364589000
Ti	1.904082000	2.562920000	1.137505000
Ti	6.428153000	-2.096564000	-1.300626000
Ti	7.039907000	1.796443000	0.014187000
Ti	4.960719000	2.949288000	2.203319000
Ti	4.003087000	0.138491000	0.076919000
Ti	3.004020000	-2.637477000	-1.578532000
Ti	3.594425000	-3.020549000	1.678707000
Ti	4.872936000	0.464596000	3.548321000
Ti	-0.026789000	-1.402067000	-0.156794000
Ti	1.186145000	1.697039000	-1.520868000
O	7.526753000	-2.382159000	0.285275000

O	5.465991000	-1.027772000	0.030998000
O	1.232090000	-2.377131000	-0.972118000
O	4.936358000	-2.915960000	-1.789609000
O	7.637496000	1.794589000	-1.734660000
O	6.802934000	-0.746679000	-2.346035000
O	1.902682000	0.934081000	-3.097481000
O	2.256544000	-2.617771000	2.931526000
O	6.276401000	-0.565678000	3.234803000
O	5.349756000	-2.751401000	1.977310000
O	7.434392000	0.375243000	0.899201000
O	0.319260000	0.273279000	-0.954013000
O	2.738503000	-2.280932000	-3.319277000
O	3.250724000	-3.699878000	0.119495000
O	0.361786000	-1.175802000	1.552796000
O	3.335874000	-0.743577000	-1.445629000
O	4.690036000	0.132546000	-3.679467000
O	1.615119000	1.147969000	2.065908000
O	2.326546000	3.427820000	-2.347602000
O	6.428258000	3.140685000	1.150877000
O	4.621417000	4.438127000	-1.064131000
O	5.323881000	1.364081000	-0.925413000
O	3.211405000	-0.190263000	3.833561000
O	3.315355000	3.592898000	1.809899000
O	4.598835000	1.120561000	1.728804000
O	5.340779000	2.650705000	-3.124920000
O	5.211093000	2.262162000	3.862819000
O	0.659783000	2.888961000	-0.171642000
O	3.157093000	-1.130095000	1.198285000
O	2.829837000	1.674313000	-0.394521000
O	-2.069817000	-0.986203000	-0.429646000
O	-1.363241000	-3.007835000	-0.026090000
H	1.989506000	4.281338000	-2.025587000
C	-8.320917000	-2.867602000	0.034258000
C	-8.659040000	-1.515608000	-0.092851000
S	-7.218806000	-0.551734000	-0.263028000
C	-6.168565000	-1.967291000	-0.167644000
C	-6.947300000	-3.118989000	-0.005495000
H	-9.061100000	-3.652077000	0.134397000
H	-6.522117000	-4.111857000	0.070304000
C	-4.770465000	-1.776166000	-0.242613000
H	-4.430122000	-0.755300000	-0.399494000
C	-3.737790000	-2.689717000	-0.127967000
C	-3.922481000	-4.082977000	0.095978000
N	-4.076180000	-5.224410000	0.276882000
C	-2.358361000	-2.216253000	-0.202436000
C	-12.588616000	0.235030000	0.000107000
C	-12.375176000	-1.107762000	0.382755000
C	-11.471475000	0.985045000	-0.430096000
H	-13.208738000	-1.705858000	0.732442000
H	-11.605006000	2.011284000	-0.752314000
C	-11.108184000	-1.665220000	0.343082000
C	-10.208341000	0.419564000	-0.463340000
H	-10.985114000	-2.690154000	0.677377000
H	-9.382269000	1.026292000	-0.824455000
C	-9.984071000	-0.919730000	-0.076855000
N	-13.865631000	0.806482000	0.047169000
C	-15.037944000	-0.000670000	-0.093142000
C	-16.090975000	0.127118000	0.824475000

C	-15.155120000	-0.906458000	-1.158172000
C	-17.246057000	-0.640471000	0.674310000
C	-16.306943000	-1.681988000	-1.291866000
C	-17.358212000	-1.551057000	-0.379988000
H	-15.999603000	0.826242000	1.649857000
H	-14.346898000	-0.995769000	-1.877433000
H	-18.055254000	-0.533222000	1.391323000
H	-16.387272000	-2.379475000	-2.120994000
H	-18.256637000	-2.151121000	-0.491409000
C	-14.034783000	2.211320000	0.253916000
C	-13.355289000	2.866166000	1.292450000
C	-14.904778000	2.941094000	-0.569443000
C	-13.534860000	4.235184000	1.491142000
C	-15.091348000	4.306613000	-0.353493000
C	-14.405030000	4.961192000	0.673042000
H	-12.693170000	2.300949000	1.940975000
H	-15.430163000	2.435745000	-1.373769000
H	-13.003512000	4.731005000	2.298775000
H	-15.767574000	4.861275000	-0.998068000
H	-14.548393000	6.025479000	0.835421000

A2-(TiO₂)₁₅

Ti	2.357448000	-0.029011000	2.646250000
Ti	5.262487000	2.498854000	-2.227534000
Ti	7.005116000	0.145190000	-2.680450000
Ti	6.898941000	-1.593762000	1.896306000
Ti	3.699098000	-0.942943000	-3.246397000
Ti	2.976836000	2.988678000	0.581490000
Ti	6.645309000	-2.752242000	-0.726708000
Ti	7.922581000	1.168568000	-0.133994000
Ti	6.033925000	3.042136000	1.673213000
Ti	4.633037000	0.083461000	0.075331000
Ti	3.182458000	-2.750020000	-1.090968000
Ti	3.638230000	-2.569375000	2.213170000
Ti	5.495660000	0.930033000	3.468583000
Ti	0.392581000	-0.771159000	-0.079804000
Ti	2.145524000	1.781043000	-1.911209000
O	7.651601000	-2.894400000	0.944103000
O	5.867290000	-1.296163000	0.324979000
O	1.459465000	-2.084653000	-0.657578000
O	5.043660000	-3.396090000	-1.117616000
O	8.532133000	0.726744000	-1.820804000
O	7.263005000	-1.707371000	-1.984344000
O	2.803044000	0.627202000	-3.255185000
O	2.362164000	-1.718836000	3.297797000
O	6.694120000	-0.373781000	3.446368000
O	5.405716000	-2.562544000	2.543979000
O	8.043067000	-0.104042000	1.019554000
O	1.035298000	0.652614000	-1.151092000
O	3.023484000	-2.691372000	-2.878255000
O	3.184530000	-3.467587000	0.798910000
O	0.795871000	-0.274691000	1.570253000
O	3.851126000	-0.959679000	-1.287176000
O	5.377115000	-0.763413000	-3.592932000
O	2.421171000	1.854208000	1.748733000
O	3.574806000	3.105641000	-2.979660000
O	7.540873000	2.792270000	0.690023000
O	5.988178000	3.894103000	-1.794596000

O	6.170560000	0.860330000	-1.056988000
O	3.748821000	0.616530000	3.784682000
O	4.532457000	3.882217000	1.105267000
O	5.371609000	1.247409000	1.546049000
O	6.432601000	1.663791000	-3.460947000
O	6.134200000	2.680727000	3.442325000
O	1.824437000	3.272242000	-0.806000000
O	3.544931000	-0.764985000	1.363885000
O	3.742915000	1.674264000	-0.719427000
O	-1.517451000	-0.105741000	-0.588951000
O	-1.227373000	-2.045773000	0.348156000
H	3.407617000	4.050348000	-2.847487000
C	-14.245413000	0.128288000	0.021845000
C	-13.996257000	-1.167382000	0.513856000
C	-13.157478000	0.871110000	-0.472626000
H	-14.814753000	-1.755043000	0.914881000
H	-13.324260000	1.864970000	-0.872893000
C	-12.711481000	-1.693065000	0.512650000
C	-11.874787000	0.339406000	-0.468007000
H	-12.551893000	-2.681779000	0.930996000
H	-11.065360000	0.933446000	-0.882884000
C	-11.614605000	-0.954861000	0.023178000
N	-15.550048000	0.669351000	0.028345000
C	-16.676801000	-0.163531000	-0.231534000
C	-17.831765000	-0.059492000	0.559968000
C	-16.651632000	-1.088671000	-1.287640000
C	-18.941027000	-0.860906000	0.291767000
C	-17.758981000	-1.898701000	-1.537294000
C	-18.910886000	-1.787517000	-0.753931000
H	-17.854426000	0.649957000	1.380609000
H	-15.766114000	-1.166321000	-1.909962000
H	-19.827525000	-0.768179000	0.912591000
H	-17.724769000	-2.608644000	-2.358719000
H	-19.774028000	-2.414181000	-0.956314000
C	-15.752451000	2.056302000	0.286425000
C	-15.065927000	2.694950000	1.332018000
C	-16.649816000	2.799908000	-0.496730000
C	-15.266737000	4.052865000	1.577515000
C	-16.858056000	4.153290000	-0.232269000
C	-16.165753000	4.789463000	0.801466000
H	-14.379189000	2.124515000	1.948813000
H	-17.180136000	2.313907000	-1.309041000
H	-14.728018000	4.531988000	2.390025000
H	-17.555542000	4.714600000	-0.847385000
H	-16.325320000	5.844744000	1.000444000
C	-9.883064000	-2.846580000	0.133428000
C	-10.266326000	-1.522119000	0.036680000
S	-8.847536000	-0.496013000	-0.049916000
C	-7.754361000	-1.868382000	0.029261000
C	-8.479978000	-3.038774000	0.132342000
H	-10.592452000	-3.664762000	0.174436000
H	-8.017995000	-4.018573000	0.171639000
C	-6.305574000	-1.691009000	-0.013835000
C	-5.443599000	-2.707753000	0.456427000
C	-5.725248000	-0.506938000	-0.518298000
C	-4.066323000	-2.547412000	0.421786000
C	-4.348812000	-0.343097000	-0.549661000
C	-3.502671000	-1.361093000	-0.079152000

H	-5.862106000	-3.618631000	0.870515000
H	-6.360546000	0.283931000	-0.904434000
H	-3.414988000	-3.332426000	0.790963000
H	-3.914606000	0.569637000	-0.942563000
C	-2.049045000	-1.172306000	-0.106675000

A3-(TiO₂)₁₅

Ti	-0.277385000	-1.258034000	-0.104044000
Ti	-6.111281000	-0.678491000	-2.160900000
Ti	-7.205484000	0.122921000	0.474527000
Ti	-3.729308000	-2.063206000	3.218866000
Ti	-4.956318000	2.648244000	-0.430947000
Ti	-2.684535000	-1.770139000	-2.883139000
Ti	-5.047226000	0.487043000	3.255570000
Ti	-6.369106000	-2.619944000	0.875930000
Ti	-4.213299000	-4.013444000	-1.073220000
Ti	-3.635349000	-0.651472000	0.172800000
Ti	-2.817851000	2.380656000	1.437245000
Ti	-0.968274000	-0.196918000	2.484622000
Ti	-2.195717000	-3.866952000	0.914356000
Ti	-0.522951000	1.956417000	-1.271109000
Ti	-3.501584000	1.001546000	-3.017988000
O	-4.648047000	-1.062203000	4.371462000
O	-4.075450000	-0.649674000	1.993710000
O	-1.407236000	2.529017000	0.149921000
O	-4.026576000	1.896857000	2.867394000
O	-7.846328000	-1.520447000	1.028742000
O	-6.530514000	0.478978000	2.354586000
O	-4.621303000	2.269856000	-2.161460000
O	0.493035000	-0.800955000	1.468332000
O	-2.848916000	-3.706186000	2.551586000
O	-2.018969000	-1.290768000	3.457740000
O	-5.448637000	-2.801260000	2.318185000
O	-1.951970000	1.629790000	-2.461948000
O	-3.872941000	3.666707000	0.752145000
O	-1.410267000	1.477973000	2.574565000
O	0.196292000	0.357492000	-1.014403000
O	-3.779217000	1.235738000	0.235919000
O	-6.441768000	1.981950000	0.168189000
O	-1.295002000	-1.694464000	-1.875923000
O	-5.506094000	0.343784000	-3.705508000
O	-5.894106000	-3.895881000	-0.391413000
O	-6.643177000	-2.068202000	-2.827707000
O	-5.658228000	-0.982814000	-0.032679000
O	-0.669408000	-3.059287000	0.387265000
O	-3.666078000	-3.345594000	-2.668736000
O	-3.440295000	-2.635106000	0.018085000
O	-7.605163000	0.076388000	-1.277993000
O	-3.052125000	-5.088091000	-0.201702000
O	-2.856272000	-0.397936000	-4.084946000
O	-1.829061000	-0.541216000	0.712009000
O	-3.839301000	-0.531689000	-1.799192000
O	0.409875000	3.116761000	-2.748701000
O	1.236594000	3.097963000	-0.730539000
H	-5.485285000	-0.168377000	-4.527206000
C	10.745171000	-1.293390000	0.121976000
C	10.856472000	-0.694444000	1.394448000
C	9.869891000	-0.703050000	-0.813346000

H	11.505478000	-1.137356000	2.141018000
H	9.776313000	-1.129815000	-1.805209000
C	10.129898000	0.442435000	1.710317000
C	9.142046000	0.430695000	-0.486297000
H	10.219499000	0.854452000	2.710143000
H	8.501767000	0.871279000	-1.245128000
C	9.251086000	1.039655000	0.781172000
N	11.484107000	-2.443186000	-0.202303000
C	12.759984000	-2.681816000	0.393725000
C	13.061408000	-3.943223000	0.928830000
C	13.728335000	-1.666874000	0.435379000
C	14.314014000	-4.182982000	1.493489000
C	14.972247000	-1.910107000	1.017118000
C	15.273506000	-3.168427000	1.545309000
H	12.313038000	-4.728528000	0.900151000
H	13.502897000	-0.693944000	0.010969000
H	14.534676000	-5.163710000	1.904765000
H	15.713007000	-1.116224000	1.043040000
H	16.245540000	-3.356474000	1.990825000
C	10.977125000	-3.399213000	-1.134126000
C	9.658619000	-3.868524000	-1.028688000
C	11.803563000	-3.892002000	-2.155282000
C	9.174150000	-4.805121000	-1.941418000
C	11.316202000	-4.841241000	-3.053356000
C	9.999620000	-5.298981000	-2.955237000
H	9.020799000	-3.499263000	-0.232248000
H	12.822562000	-3.528816000	-2.240283000
H	8.151953000	-5.160374000	-1.848796000
H	11.965996000	-5.214399000	-3.839601000
H	9.621553000	-6.033464000	-3.659707000
C	8.753484000	3.125576000	2.173789000
C	8.496635000	2.235009000	1.135194000
S	7.073181000	2.714823000	0.239585000
C	6.832184000	4.131214000	1.263521000
C	7.830420000	4.175059000	2.241625000
H	9.599470000	3.030444000	2.843137000
H	7.873455000	4.970617000	2.977644000
C	5.811961000	5.119859000	1.199782000
H	5.936180000	5.865033000	1.984730000
C	2.578630000	6.202827000	-0.681636000
S	3.620634000	6.689110000	0.641833000
C	4.727651000	5.319213000	0.385412000
C	4.268505000	4.521316000	-0.741665000
O	4.773858000	3.506237000	-1.209027000
S	1.185303000	7.010371000	-1.103135000
N	3.086775000	5.084029000	-1.287456000
C	2.417580000	4.423383000	-2.393452000
C	1.300785000	3.513367000	-1.922691000
H	3.161254000	3.808733000	-2.908744000
H	2.017788000	5.163421000	-3.087269000

A4-(TiO₂)₁₅

Ti	0.845118000	-0.297352000	1.121977000
Ti	-4.015605000	-1.097940000	-2.685275000
Ti	-5.937299000	0.229256000	-0.861649000
Ti	-3.493184000	-0.634197000	3.322706000
Ti	-3.609949000	2.718463000	-1.770007000
Ti	-0.482051000	-1.870704000	-1.994441000

Ti	-4.848953000	1.612465000	2.185318000	C	8.503302000	-7.723499000	0.503195000
Ti	-5.196323000	-2.196321000	0.547425000	H	5.311213000	-7.009368000	1.458950000
Ti	-2.422713000	-3.725238000	-0.122055000	H	7.874928000	-4.870636000	-1.251281000
Ti	-2.454488000	-0.111388000	0.163514000	H	7.094378000	-8.691379000	1.820059000
Ti	-2.229683000	3.230780000	0.675592000	H	9.668564000	-6.535001000	-0.870264000
Ti	-0.725211000	1.282251000	2.948303000	H	9.286705000	-8.457624000	0.664242000
Ti	-1.188227000	-2.744378000	2.226450000	C	4.132764000	-5.383351000	-0.458400000
Ti	0.853387000	2.421560000	-0.959858000	C	3.008229000	-4.976139000	0.274059000
Ti	-1.328846000	0.637751000	-3.154936000	C	3.984141000	-6.311117000	-1.498915000
O	-4.799894000	0.517445000	3.763105000	C	1.746879000	-5.484643000	-0.041625000
O	-3.470649000	0.321230000	1.685823000	C	2.722844000	-6.825034000	-1.801751000
O	-0.432494000	3.235545000	-0.097301000	C	1.599940000	-6.411881000	-1.078853000
O	-3.797927000	2.998434000	1.724830000	H	3.125317000	-4.267075000	1.087628000
O	-6.673963000	-1.258500000	-0.070674000	H	4.856313000	-6.626998000	-2.062197000
O	-5.952562000	1.186388000	0.916680000	H	0.879803000	-5.166840000	0.530157000
O	-2.694720000	1.963984000	-3.120803000	H	2.618470000	-7.545667000	-2.607493000
O	1.021323000	0.662050000	2.645156000	H	0.618929000	-6.811502000	-1.318476000
O	-2.365108000	-2.231851000	3.449769000	C	7.538639000	1.397488000	0.610016000
O	-2.014995000	0.389354000	3.853740000	C	6.393633000	0.729565000	0.173634000
O	-4.789220000	-1.832734000	2.169855000	S	5.146831000	1.872634000	-0.245751000
O	-0.075334000	1.612432000	-2.369767000	C	6.181003000	3.246130000	0.132172000
O	-3.010902000	4.144733000	-0.653803000	C	7.418422000	2.790377000	0.595913000
O	-1.221437000	2.844270000	2.401022000	H	8.446262000	0.884166000	0.900515000
O	1.503866000	1.040849000	-0.032633000	H	8.223309000	3.460052000	0.877184000
O	-2.668844000	1.692552000	-0.376074000	C	5.461398000	8.387458000	0.960267000
O	-5.172998000	2.036915000	-1.480023000	C	5.481822000	7.046700000	0.574823000
O	0.504293000	-1.356174000	-0.699664000	C	4.616741000	6.556268000	-0.414949000
O	-2.970886000	-0.430119000	-4.184933000	C	3.691542000	7.402271000	-1.035465000
O	-4.234809000	-3.677169000	-0.058306000	C	3.669327000	8.738744000	-0.646615000
O	-4.271691000	-2.661337000	-3.071870000	C	4.543778000	9.228581000	0.336548000
O	-4.269769000	-0.777411000	-0.532209000	C	5.765321000	4.607782000	0.108648000
O	0.411261000	-1.954872000	1.967293000	N	4.824710000	5.188901000	-0.672724000
O	-1.420777000	-3.443837000	-1.600483000	H	6.134998000	8.758500000	1.724285000
O	-2.121276000	-2.002010000	0.677255000	H	3.003330000	7.041851000	-1.790376000
O	-5.734747000	-0.325728000	-2.558728000	H	2.958560000	9.411000000	-1.114916000
O	-1.554047000	-4.335327000	1.348548000	H	4.502689000	10.274984000	0.619149000
O	-0.307406000	-0.871677000	-3.535542000	S	6.478557000	5.753088000	1.211564000
O	-0.939672000	0.342931000	1.198585000	C	4.156914000	4.527451000	-1.793821000
O	-1.969236000	-0.544737000	-1.706423000	C	2.837243000	3.872584000	-1.419221000
O	2.138483000	3.343000000	-2.346649000	H	4.817544000	3.763164000	-2.209067000
O	2.449443000	3.785328000	-0.225033000	H	3.990990000	5.258209000	-2.587057000
H	-2.662950000	-1.123561000	-4.786889000	A5-(TiO ₂) ₁₅			
C	5.670092000	-3.503678000	-0.062923000	Ti	2.147837000	-1.517422000	2.432154000
C	6.730595000	-2.982480000	0.713739000	Ti	3.669291000	3.378479000	-0.963832000
C	4.855872000	-2.587505000	-0.768090000	Ti	5.703022000	1.966909000	-2.632922000
H	7.362922000	-3.655779000	1.279850000	Ti	7.287903000	-0.964072000	0.691002000
H	4.047477000	-2.953349000	-1.389704000	Ti	2.779390000	0.373476000	-3.292412000
C	6.962655000	-1.619014000	0.777949000	Ti	2.012570000	2.031668000	1.937944000
C	5.094157000	-1.226044000	-0.695258000	Ti	6.381125000	-1.478997000	-1.993397000
H	7.768004000	-1.259382000	1.410047000	Ti	6.870174000	2.299242000	-0.021220000
H	4.464473000	-0.561707000	-1.280413000	Ti	5.111470000	2.406215000	2.718424000
C	6.151526000	-0.698600000	0.078138000	Ti	4.054418000	0.100509000	0.065925000
N	5.433188000	-4.877619000	-0.135421000	Ti	2.888922000	-2.229303000	-2.086280000
C	6.480339000	-5.827041000	0.087703000	Ti	3.683335000	-3.390565000	0.872815000
C	6.264767000	-6.911298000	0.950225000	Ti	5.314662000	-0.382963000	3.303445000
C	7.712143000	-5.700790000	-0.571563000	Ti	-0.094837000	-1.606937000	-0.180494000
C	7.271596000	-7.855725000	1.149530000	Ti	0.942987000	1.828512000	-0.753309000
C	8.718774000	-6.641632000	-0.354657000				

O	7.792756000	-1.930406000	-0.706831000	C	-12.606307000	4.406508000	1.468230000
O	5.672039000	-0.795733000	-0.273900000	C	-14.194420000	4.788096000	-0.306457000
O	1.221881000	-2.106657000	-1.385820000	C	-13.351031000	5.293826000	0.686502000
O	4.911490000	-2.320408000	-2.420398000	H	-12.137485000	2.345359000	1.888576000
O	7.206772000	2.707862000	-1.748253000	H	-14.934031000	3.027337000	-1.306238000
O	6.484191000	0.145137000	-2.670122000	H	-11.952727000	4.784573000	2.249213000
O	1.671456000	1.551892000	-2.485948000	H	-14.774319000	5.466155000	-0.926146000
O	2.587292000	-3.313160000	2.341554000	H	-13.275490000	6.364610000	0.849133000
O	6.554842000	-1.383283000	2.342063000	C	-8.806588000	-3.477497000	0.316650000
O	5.441277000	-3.733646000	1.168587000	C	-8.926255000	-2.125013000	0.074109000
O	7.727879000	0.799839000	0.462856000	S	-7.333513000	-1.435550000	-0.206031000
O	0.189660000	0.294800000	-0.542885000	C	-6.528853000	-2.983752000	0.016408000
O	2.541527000	-1.455188000	-3.687154000	C	-7.470112000	-3.955444000	0.288045000
O	3.238082000	-3.713810000	-0.784100000	H	-9.658271000	-4.121557000	0.504246000
O	0.603138000	-1.677064000	1.516684000	H	-7.211990000	-4.990938000	0.477770000
O	3.315436000	-0.382288000	-1.557809000	C	-5.071460000	-3.104546000	-0.087613000
O	4.299480000	1.082210000	-3.748708000	C	-4.468462000	-4.373443000	-0.215577000
O	1.873756000	0.420295000	2.601038000	C	-4.244209000	-1.957242000	-0.054139000
O	1.780769000	3.801311000	-1.180797000	H	-5.092200000	-5.259455000	-0.270567000
O	6.341065000	3.106880000	1.542006000	H	-4.665069000	-0.962101000	0.054695000
O	4.218828000	4.641803000	-0.086663000	C	-3.079588000	-4.522502000	-0.291000000
O	5.152525000	1.740598000	-0.745591000	C	-2.865971000	-2.102771000	-0.137623000
O	3.814889000	-1.160701000	3.630943000	H	-2.630239000	-5.506377000	-0.389769000
O	3.412578000	3.009867000	2.712375000	C	-2.274870000	-3.383757000	-0.247826000
O	4.775918000	0.754381000	1.810091000	H	5.884842000	-3.318707000	1.932409000
O	4.622006000	3.408189000	-2.582463000				
O	5.595972000	1.308381000	4.069832000	A6-(TiO ₂) ₁₅			
O	0.584307000	2.562271000	0.995688000	Ti	4.240951000	-0.299044000	-2.798132000
O	3.345507000	-1.426687000	0.912456000	Ti	6.987635000	-2.023558000	2.462042000
O	2.740136000	1.623358000	0.149678000	Ti	8.194481000	0.637814000	2.983427000
O	-1.963510000	-1.106033000	-0.114102000	Ti	8.265975000	2.178318000	-1.707136000
O	-0.935144000	-3.338189000	-0.305900000	Ti	4.694392000	1.081753000	3.121991000
H	1.463648000	4.520894000	-0.615654000	Ti	5.190221000	-3.055257000	-0.549138000
C	-12.482032000	0.312007000	0.046190000	Ti	7.527415000	3.329261000	0.813087000
C	-12.482200000	-0.968712000	0.628782000	Ti	9.579458000	-0.290367000	0.613125000
C	-11.289424000	0.775600000	-0.535695000	Ti	8.298045000	-2.541806000	-1.316422000
H	-13.385736000	-1.343657000	1.097517000	Ti	6.199231000	0.131473000	-0.017209000
H	-11.266340000	1.753808000	-1.003721000	Ti	4.140053000	2.678064000	0.816232000
C	-11.333790000	-1.749786000	0.630045000	Ti	4.945624000	2.464906000	-2.397912000
C	-10.143057000	-0.009666000	-0.526904000	Ti	7.582633000	-0.615871000	-3.255334000
H	-11.363735000	-2.719438000	1.116840000	Ti	1.883241000	0.141702000	-0.359482000
H	-9.247360000	0.376262000	-1.005465000	Ti	3.854312000	-1.957575000	1.768649000
C	-10.130411000	-1.293037000	0.053919000	O	8.676021000	3.614656000	-0.722222000
N	-13.648046000	1.115416000	0.051633000	O	7.162584000	1.722898000	-0.235926000
C	-14.927616000	0.525231000	-0.148083000	O	2.634951000	1.616691000	0.251290000
C	-16.021255000	0.913410000	0.643402000	O	5.791064000	3.682238000	0.979628000
C	-15.116520000	-0.449618000	-1.141786000	O	9.881706000	0.347332000	2.343056000
C	-17.276185000	0.341407000	0.437373000	O	8.141667000	2.467955000	2.204129000
C	-16.371032000	-1.029011000	-1.328584000	O	4.120781000	-0.637967000	3.085186000
C	-17.459266000	-0.635640000	-0.544919000	O	4.003825000	1.345465000	-3.551540000
H	-15.882168000	1.661276000	1.417129000	O	8.537391000	0.891673000	-3.145932000
H	-14.279368000	-0.747299000	-1.764597000	O	6.714869000	2.822726000	-2.547327000
H	-18.111153000	0.652841000	1.058608000	O	9.585938000	0.936236000	-0.572353000
H	-16.499714000	-1.781093000	-2.101807000	O	2.609240000	-1.133931000	0.831290000
H	-18.436302000	-1.083581000	-0.698031000	O	3.766547000	2.661604000	2.565121000
C	-13.546334000	2.519803000	0.264584000	O	4.152457000	3.307116000	-1.102965000
C	-12.706794000	3.030103000	1.268589000	O	2.547402000	-0.335992000	-1.939379000
C	-14.288059000	3.413924000	-0.524767000	O	5.107169000	1.063911000	1.200764000

O	6.304496000	1.245716000	3.693781000	C	-8.352269000	-1.727494000	0.032115000
O	4.561928000	-2.097819000	-1.838964000	C	-8.876790000	0.536602000	-0.682565000
O	5.365900000	-2.936079000	3.056441000	H	-8.634859000	-2.719470000	0.364820000
O	9.597496000	-1.975431000	-0.189356000	H	-9.614283000	1.287458000	-0.946944000
O	8.022048000	-3.255231000	2.190204000	C	-6.982105000	-1.426264000	-0.039634000
O	7.698711000	-0.287597000	1.316054000	C	-7.543960000	0.852267000	-0.754594000
O	5.859883000	-0.680627000	-3.758259000	H	-7.230995000	1.845622000	-1.061505000
O	6.938787000	-3.644134000	-0.856595000	C	-6.555201000	-0.120853000	-0.441386000
O	7.284487000	-0.914139000	-1.343230000	C	-4.810265000	-2.115000000	0.237837000
O	7.803192000	-0.938541000	3.769597000	C	-4.242082000	-0.851512000	-0.167252000
O	8.526140000	-2.202315000	-3.086772000	C	-5.175848000	0.132904000	-0.501043000
O	3.975028000	-3.527572000	0.725503000	H	-4.842362000	1.120561000	-0.796555000
O	5.106848000	0.707775000	-1.450274000	N	-6.070993000	-2.396916000	0.295495000
O	5.522341000	-1.570518000	0.746474000	C	-2.812651000	-0.652125000	-0.181018000
O	-0.014742000	-0.626546000	0.112319000	C	-2.053876000	0.343225000	-0.731781000
O	0.166661000	1.153544000	-1.135452000	C	-2.548103000	1.441890000	-1.498365000
H	5.401483000	-3.897499000	2.944819000	N	-2.931699000	2.342930000	-2.128478000
C	-17.404283000	0.138280000	0.104545000	C	-0.584617000	0.289873000	-0.578597000
C	-16.999100000	-1.176447000	0.406276000	H	-2.224601000	-1.417756000	0.313767000
C	-16.417180000	1.065388000	-0.279492000	Cl	-3.723862000	-3.445941000	0.685595000
H	-17.737310000	-1.905734000	0.721094000	A7-(TiO ₂) ₁₅			
H	-16.703776000	2.080026000	-0.532627000	Ti	4.504861000	-0.998350000	-2.764877000
C	-15.663729000	-1.544349000	0.326630000	Ti	6.626629000	-1.396068000	3.033627000
C	-15.082877000	0.690097000	-0.355177000	Ti	7.752464000	1.344837000	3.053904000
H	-15.386404000	-2.557717000	0.598263000	Ti	8.386157000	1.781365000	-1.846650000
H	-14.355091000	1.427279000	-0.682473000	Ti	4.262580000	1.719455000	2.684521000
C	-14.667288000	-0.622622000	-0.056408000	Ti	5.185542000	-3.129151000	0.155270000
N	-18.761492000	0.515582000	0.186256000	Ti	7.373392000	3.438336000	0.266637000
C	-19.788608000	-0.403573000	-0.177683000	Ti	9.436220000	-0.069919000	1.166615000
C	-20.930295000	-0.544851000	0.627081000	Ti	8.377816000	-2.738089000	-0.346906000
C	-19.677561000	-1.168844000	-1.349818000	Ti	6.142076000	0.111064000	0.047621000
C	-21.942460000	-1.430824000	0.259326000	Ti	4.007638000	2.727516000	0.016995000
C	-20.686529000	-2.065310000	-1.700404000	Ti	5.181884000	1.791252000	-2.943191000
C	-21.825768000	-2.199074000	-0.902102000	Ti	7.880316000	-1.324904000	-2.740121000
H	-21.018931000	0.040699000	1.536223000	Ti	1.890459000	-0.065306000	-0.778094000
H	-18.802628000	-1.055822000	-1.981541000	Ti	3.603516000	-1.561458000	1.995662000
H	-22.819922000	-1.529226000	0.891962000	O	8.686334000	3.408474000	-1.155480000
H	-20.586772000	-2.649801000	-2.610505000	O	7.132176000	1.625095000	-0.434566000
H	-22.612981000	-2.892249000	-1.182267000	O	2.600417000	1.528952000	-0.469763000
C	-19.121289000	1.819055000	0.637533000	O	5.636300000	3.782887000	0.134550000
C	-18.502919000	2.378208000	1.767521000	O	9.500725000	0.966017000	2.731719000
C	-20.108995000	2.554384000	-0.036783000	O	7.816965000	2.948117000	1.882923000
C	-18.860841000	3.653295000	2.204187000	O	3.709173000	0.022514000	3.004389000
C	-20.473205000	3.821522000	0.417604000	O	4.351026000	0.424841000	-3.900343000
C	-19.849658000	4.380679000	1.536203000	O	8.849781000	0.174149000	-2.830351000
H	-17.746970000	1.810410000	2.300099000	O	6.970272000	2.146503000	-2.990877000
H	-20.586963000	2.129256000	-0.913209000	O	9.590150000	0.867795000	-0.237562000
H	-18.373995000	4.071961000	3.080299000	O	2.492247000	-0.998867000	0.754543000
H	-21.239304000	4.378155000	-0.114476000	O	3.426419000	3.110698000	1.659859000
H	-20.131277000	5.369928000	1.883696000	O	4.271524000	2.912349000	-1.989037000
C	-12.739234000	-2.308991000	-0.184271000	O	2.711588000	-0.878624000	-2.124879000
C	-13.265850000	-1.030082000	-0.131877000	O	4.921792000	1.271251000	0.887507000
S	-11.969429000	0.149181000	-0.145792000	O	5.791166000	2.060540000	3.378475000
C	-10.733694000	-1.096567000	-0.234205000	O	4.700875000	-2.510007000	-1.382040000
C	-11.327701000	-2.345224000	-0.238405000	O	4.945473000	-2.191545000	3.630768000
H	-13.354346000	-3.200300000	-0.213810000	O	9.527239000	-1.896661000	0.766932000
H	-10.762832000	-3.267040000	-0.315343000	O	7.685051000	-2.629944000	3.183078000
C	-9.315206000	-0.768748000	-0.291461000				

O	7.469112000	0.045084000	1.608767000	C	-7.560231000	0.445226000	-1.507439000
O	6.221935000	-1.537403000	-3.412513000	H	-7.251056000	1.317024000	-2.075830000
O	6.959131000	-3.716350000	0.206263000	C	-6.562933000	-0.416113000	-0.985243000
O	7.368065000	-1.186400000	-0.861451000	C	-4.640944000	-2.199652000	0.185693000
O	7.257090000	-0.013237000	4.140809000	C	-4.216450000	-1.015124000	-0.596966000
O	8.791128000	-2.807424000	-2.117613000	C	-5.176846000	-0.183374000	-1.149356000
O	3.835193000	-3.329365000	1.354674000	H	-4.875841000	0.691669000	-1.715687000
O	5.218187000	0.317183000	-1.601796000	N	-6.010882000	-2.379169000	0.285552000
O	5.378261000	-1.382024000	1.108797000	H	-6.292749000	-3.194113000	0.819042000
O	-0.016809000	-0.778167000	-0.310775000	C	-2.796991000	-0.830545000	-0.664573000
O	0.237877000	0.737494000	-1.855644000	C	-2.012456000	0.049141000	-1.366531000
H	4.992714000	-3.151618000	3.748412000	C	-2.492654000	1.020674000	-2.293904000
C	-17.345778000	0.145129000	0.251637000	N	-2.878581000	1.816332000	-3.052625000
C	-16.927553000	-1.112534000	0.728106000	C	-0.553844000	0.000297000	-1.178117000
C	-16.383466000	0.982922000	-0.342887000	O	-3.870445000	-2.998310000	0.722221000
H	-17.645450000	-1.770040000	1.205674000	H	-2.240802000	-1.527025000	-0.043232000
H	-16.680936000	1.950855000	-0.730684000				
C	-15.603988000	-1.511615000	0.613477000	A8-(TiO ₂) ₁₅			
C	-15.060705000	0.576456000	-0.453441000	Ti	3.140842000	-2.675010000	0.195944000
H	-15.314982000	-2.474399000	1.021994000	Ti	3.885740000	3.515973000	1.610749000
H	-14.354389000	1.241711000	-0.942132000	Ti	6.330312000	3.834727000	0.022327000
C	-14.632105000	-0.679917000	0.018922000	Ti	7.756906000	-0.828224000	-0.126768000
N	-18.690822000	0.554270000	0.370118000	Ti	3.691047000	3.119436000	-2.138623000
C	-19.746621000	-0.393585000	0.233645000	Ti	2.261200000	0.295384000	2.348139000
C	-20.823446000	-0.391027000	1.134487000	Ti	7.425717000	1.271972000	-2.012802000
C	-19.727559000	-1.334288000	-0.808739000	Ti	7.139283000	1.923979000	1.991835000
C	-21.861541000	-1.310971000	0.989252000	Ti	5.145295000	0.225932000	3.742364000
C	-20.761214000	-2.261535000	-0.935880000	Ti	4.689439000	0.547001000	0.110906000
C	-21.835304000	-2.253870000	-0.041822000	Ti	4.314779000	0.600935000	-3.257288000
H	-20.841294000	0.331052000	1.944156000	Ti	5.208358000	-2.214039000	-1.789370000
H	-18.904516000	-1.332892000	-1.515899000	Ti	5.809212000	-2.038656000	2.220036000
H	-22.687637000	-1.297181000	1.694410000	Ti	1.222382000	-0.666998000	-2.016276000
H	-20.732619000	-2.982759000	-1.747596000	Ti	1.466262000	2.078401000	0.235082000
H	-22.642098000	-2.972528000	-0.148078000	O	8.720444000	-0.003982000	-1.389723000
C	-19.008098000	1.917447000	0.640732000	O	6.397176000	0.378361000	-0.657197000
C	-18.306573000	2.629882000	1.626700000	O	2.551376000	-0.117335000	-3.036749000
C	-20.035735000	2.559805000	-0.067851000	O	6.213653000	1.017771000	-3.289775000
C	-18.622665000	3.962750000	1.887616000	O	7.615617000	3.553164000	1.334688000
C	-20.356591000	3.887884000	0.211878000	O	7.444202000	2.880994000	-1.347185000
C	-19.650713000	4.598554000	1.186354000	O	2.304150000	3.267407000	-0.991816000
H	-17.519037000	2.135677000	2.186279000	O	4.013410000	-3.496172000	-1.155479000
H	-20.577942000	2.015476000	-0.834144000	O	7.360848000	-2.013401000	1.399219000
H	-18.071667000	4.500330000	2.653966000	O	6.904424000	-2.122656000	-1.207208000
H	-21.154208000	3.671507000	-0.344690000	O	8.030991000	0.618158000	1.296092000
H	-19.899238000	5.634094000	1.397422000	O	0.964707000	0.870159000	-0.936843000
C	-12.723243000	-2.390743000	0.082108000	O	3.765328000	2.230026000	-3.800991000
C	-13.242026000	-1.118401000	-0.086626000	O	4.893040000	-1.307135000	-3.240385000
S	-11.948114000	0.010539000	-0.440177000	O	1.787721000	-1.908730000	-0.895723000
C	-10.725563000	-1.248160000	-0.359840000	O	4.183947000	1.364136000	-1.507758000
C	-11.319914000	-2.461201000	-0.064854000	O	5.066136000	3.995470000	-1.600932000
H	-13.339411000	-3.258936000	0.282358000	O	2.352092000	-1.252632000	1.646986000
H	-10.763510000	-3.388555000	0.007297000	O	1.932950000	3.778830000	1.485058000
C	-9.314062000	-0.961358000	-0.573843000	O	6.423635000	1.504505000	3.659537000
C	-8.339242000	-1.821758000	-0.047169000	O	4.102217000	3.471367000	3.212153000
C	-8.896421000	0.185407000	-1.308194000	O	5.531978000	2.285100000	0.871506000
H	-8.630792000	-2.680495000	0.547769000	O	4.475868000	-3.001261000	1.520405000
H	-9.640956000	0.849152000	-1.734320000	O	3.357841000	0.492344000	3.852974000
C	-6.982729000	-1.558190000	-0.245653000	O	5.211339000	-0.219875000	1.888808000

O	5.104172000	4.788129000	0.891002000	H	-11.121026000	-0.200517000	2.042299000
O	5.713615000	-1.464773000	3.992657000	H	-11.709561000	0.106044000	-2.215408000
O	0.823790000	1.294475000	1.822121000	C	-11.220693000	-0.125416000	-0.119086000
O	4.314503000	-1.139201000	-0.449329000	N	-15.157462000	1.343544000	0.531904000
O	3.155445000	1.413335000	0.976384000	C	-15.919246000	0.907893000	1.657985000
O	-0.951844000	-0.837664000	-2.061663000	C	-16.608506000	1.841339000	2.446145000
O	0.344144000	-1.878696000	-3.479750000	C	-16.001986000	-0.456067000	1.977154000
H	1.509547000	3.765206000	2.356078000	C	-17.368955000	1.413122000	3.533085000
C	-4.251119000	-2.031733000	-2.936491000	C	-16.751048000	-0.873290000	3.076156000
C	-5.264743000	-1.989142000	-1.886514000	C	-17.440844000	0.056615000	3.857293000
S	-4.666057000	-2.697898000	-0.385433000	H	-16.545159000	2.896344000	2.200541000
C	-3.095551000	-3.042048000	-1.125733000	H	-15.480772000	-1.181468000	1.360932000
O	-4.334712000	-1.621905000	-4.081601000	H	-17.897870000	2.146034000	4.135446000
N	-3.066654000	-2.651053000	-2.438785000	H	-16.807460000	-1.932070000	3.312097000
C	-1.913625000	-2.692004000	-3.326958000	H	-18.029555000	-0.272572000	4.708021000
C	-0.798242000	-1.736549000	-2.936318000	C	-15.744068000	2.281387000	-0.370767000
C	0.079992000	-4.234660000	0.751212000	C	-15.021939000	3.405762000	-0.798818000
S	-0.446798000	-4.045920000	-0.892128000	C	-17.058209000	2.094546000	-0.824247000
C	-2.089597000	-3.629179000	-0.381721000	C	-15.604049000	4.317774000	-1.677718000
C	-2.219207000	-3.803331000	1.051093000	C	-17.637915000	3.020967000	-1.689602000
S	1.695116000	-4.570286000	1.186407000	C	-16.914311000	4.133324000	-2.124801000
N	-0.947329000	-4.135644000	1.616898000	H	-14.009661000	3.559701000	-0.439355000
O	-3.217799000	-3.657651000	1.744185000	H	-17.617303000	1.225201000	-0.494064000
C	-0.819364000	-4.235504000	3.084457000	H	-15.034538000	5.184215000	-2.001354000
H	-1.788960000	-4.592292000	3.435928000	H	-18.656328000	2.864827000	-2.033408000
H	-0.059146000	-4.988954000	3.294597000	H	-17.367010000	4.849849000	-2.803266000
C	-0.465461000	-2.890895000	3.720145000	C	-9.065746000	-1.322650000	0.576908000
H	-1.241740000	-2.149260000	3.512214000	C	-9.870981000	-0.633928000	-0.324922000
H	0.493690000	-2.525592000	3.343623000	S	-9.025603000	-0.420873000	-1.835489000
H	-0.389708000	-3.014376000	4.805031000	C	-7.599967000	-1.271290000	-1.249351000
H	-1.507946000	-3.702985000	-3.417951000	C	-7.805889000	-1.675903000	0.067667000
H	-2.289103000	-2.398010000	-4.313068000	H	-9.396225000	-1.588441000	1.573536000
C	-13.856550000	0.858415000	0.316199000	H	-7.075107000	-2.228490000	0.645573000
C	-13.024938000	0.505071000	1.398839000	C	-6.486527000	-1.428412000	-2.123298000
C	-13.342669000	0.711724000	-0.988385000	H	-6.593794000	-1.047975000	-3.138113000
H	-13.387859000	0.626822000	2.412979000				
H	-13.965746000	0.960627000	-1.839711000				
C	-11.743030000	0.026211000	1.182323000				
C	-12.058073000	0.233959000	-1.194270000				