

Supporting Information

Exploring Isomeric Effects on Optical and Electrochemical Properties of Red/Orange Electrochromic Polymers

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Materials and Methods

All chemicals were purchased from commercial sources and used as received unless otherwise noted. *N,N*-dimethylacetamide was degassed with argon for 15 minutes and stored over molecular sieves (4Å, 1-2 mm beads) prior to use. 60 Å silica gel (230-400 mesh) was used for all column chromatography. ¹H NMR and ¹³C NMR spectra were collected on a Bruker Avance III HD 500 MHz NMR spectrometer with nominal concentrations of 10-15 mg/mL in CDCl₃, peaks are referenced to the residual CHCl₃ peak (¹H: δ = 7.26 ppm; ¹³C: δ = 77.23 ppm). Polymer molecular weights were estimated via size exclusion chromatography (SEC) using a Tosoh EcoSEC HLC-8320 operated at 40 °C while using chloroform as the eluent. Polymer solutions (~5 mg/mL in CHCl₃) were prepared and filtered through a PTFE 0.45 μm filter prior to injection. Differential scanning calorimetry (DSC) measurements were made using a TA instruments Q-200 DSC with a heat-cool-heat cycle from 0 °C to 270 °C at a heating rate of 10 °C/min. Thermal transition values were obtained from the second heating cycle. Optical absorption spectra were acquired using a Varian Cary 5000 Scan dual-beam UV-vis-near-IR spectrophotometer. Spectra acquired from

this same spectrophotometer was used to extract colorimetry data calculated using Star-Tek colorimetry software using a D50 illuminant, 2 deg observer, and the CIELAB $L^*a^*b^*$ color space. Electrochemical measurements were performed using an EG&G Princeton Applied Research model 273A potentiostat/galvanostat under CorrWare control in a three-electrode cell configuration, using ITO/glass (Delta Technologies Inc., $7 \times 50 \times 0.7$ mm, sheet resistance, R_s , 8–12 Ω/sq) as the working electrode, a Ag/Ag⁺ reference electrode (calibrated versus ferrocene, $E_{1/2} = 62.5$ mV), and a Pt flag as the counter electrode, with a 50 mV/s scan rate. The ITO slides were cleaned by sequential sonication in acetone, acetonitrile, and isopropanol. Surfaces were thoroughly rinsed with each solvent after each respective cycle. Films were subsequently exposed to a 5 min phosphonic acid treatment (10.0 mM hexadecylphosphonic acid in ethanol). An electrolyte solution of 0.5 M tetrabutylammonium hexafluorophosphate (TBAPF₆, 98%, purified via recrystallization from hot ethanol) in propylene carbonate (PC) was used in all electrochemical and spectroelectrochemical measurements. PC was purified using a Vacuum Atmospheres solvent purifier. Electrochromic polymer films were spray-cast onto the ITO-coated glass slides using an Iwata airbrush at 20 psi from 5 mg/mL chloroform solutions. Photography was performed in a light booth designed to exclude outside light with a D50 (5000K) lamp located in the back of the booth providing illumination, using a Nikon D90 SLR camera with a Nikon 18-105 mm VR lens. Pictures are presented without manipulation except for cropping.

Computational Treatment & Results

The functional and basis set mPW1PBE/cc-PVDZ include the following details. With respect to mPW1PBE, this *one*-parameter, hybrid functional is a variation of the *Perdew-Wang* exchange with *PBE* correlation. The basis set, cc-PVDZ, is a correlation consistent (cc), *double-zeta* basis set which includes valence *polarization* functions (PV) for specific atoms.

I. Keywords for calculations:

- A. DFT: opt freq cc-pvdz scrf=(cpcm,solvent=dichloromethane) geom=connectivity mpw1pbe scf=qc int=superfine
- B. TDDFT: td=(nstates=15)/cc-pvdz scrf=(cpcm,solvent=dichloromethane) scf=qc geom=connectivity mpw1pbe

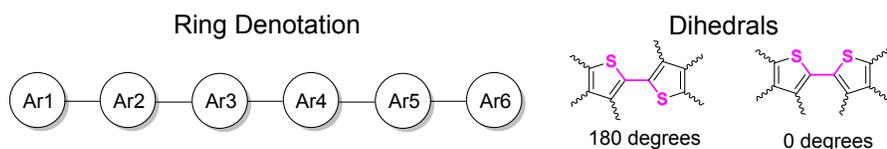


Figure S1: Legend for dihedral angle study with definitions for 180 and 0 degrees.

Table S1: Here the optical properties, dihedral angles as well as the color for each hexamer in its neutral state is provided.

CCE	Neutral Properties											
	HOMO (eV)	LUMO (eV)	Band Gap (eV)	Dihedral					Color			
				AR ₁ -AR ₂	AR ₂ -AR ₃	AR ₃ -AR ₄	AR ₄ -AR ₅	AR ₅ -AR ₆	R	G	B	Swatch
DPDPDP	-5.03	-1.94	2.50	161.1	160.6	162.8	164.1	131.8	168	84	92	
DRDRDR	-5.01	-1.96	2.47	154.8	162.4	158.2	159.9	156.8	159	77	99	
DSDSDS	-5.13	-1.83	2.67	132.9	177.8	138.3	168.7	130.3	198	123	57	
DSDSDT	-5.17	-1.78	2.74	132.0	172.3	129.6	173.0	133.0	203	134	50	
DSDADS	-5.10	-1.86	2.62	122.0	179.0	156.1	144.9	150.9	192	112	65	
DSDADA	-5.23	-1.73	2.84	122.7	175.0	123.7	171.7	131.9	205	159	55	
DADADA	-5.21	-1.74	2.67	122.2	175.9	124.6	173.2	134.5	205	154	52	

Table S2: Dihedrals as well as color are provided for the hexamers in their radical cation states.

CCE	Radical Cation Properties								
	Dihedral					Color			
	AR ₁ -AR ₂	AR ₂ -AR ₃	AR ₃ -AR ₄	AR ₄ -AR ₅	AR ₅ -AR ₆	R	G	B	Swatch
DPDPDP	171.6	172.9	176.5	175.6	168.9	0	157	186	
DRDRDR	171.0	177.1	173.5	179.7	168.6	0	157	186	
DSDSDS	140.4	176.7	160	164.4	166.2	0	144	185	
DSDSDA	145.9	170.3	166.3	171.2	159.6	0	151	186	
DSDADS	157.6	173.3	158.8	161.5	165.3	0	148	184	
DSDADA	153.3	171.9	164.9	171.8	161.6	0	154	181	
DADADA	133.8	179.3	163.8	173.2	159.8	0	147	185	

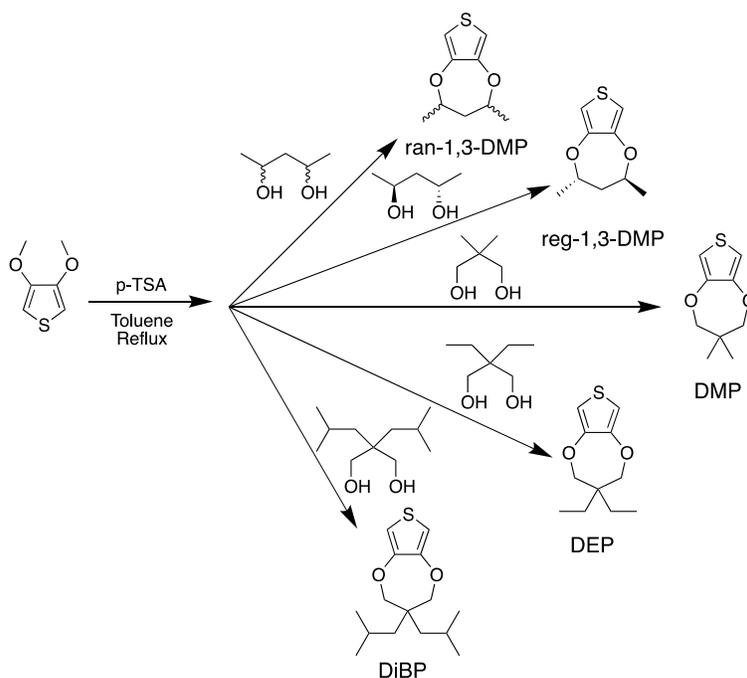
Table S3: Neutral excited states with oscillator strengths (f) of 0.1000 and above are given for each hexamer along with the transitions from which they originated as well as their corresponding wavelengths.

CCE	Neutral Excited States								
	ES1			ES2			ES3		
	λ (nm)	f	transition	λ (nm)	f	transition	λ (nm)	f	transition
DPDPDP	495.0	1.9365	H→L	320.0	0.2299	H-1→L+1 H→L+2	N/A	N/A	N/A
DRDRDR	502.2	1.9539	H→L	326.9	0.2800	H-1→L+1	N/A	N/A	N/A
DSDSDS	464.3	1.7481	H→1	325.0	0.2248	H-1→L+1 H→L+2	319.0	0.1066	H→L+2 H-1→L+1 H→L+2
DSDSDA	452.5	1.7237	H→1	328.4	0.3531	H-1→L+1	N/A	N/A	N/A
DSDADS	427.2	1.7997	H→1	319.8	0.2546	H-1→L+1 H→L+2	N/A	N/A	N/A
DSDADA	436.4	1.6535	H→1	327.2	0.387	H-1→L+1	N/A	N/A	N/A
DADADA	440.5	1.6713	H→1	327.5	0.3827	H-1→L+1	N/A	N/A	N/A

Table S4: Radical cation excited states with oscillator strengths (f) of 0.7900 and above are given for each hexamer along with the transitions from which they originated as well as their corresponding wavelengths.

CCE	Radical Cation Excited States					
	ES1			ES2		
	λ (nm)	f	transition	λ (nm)	f	transition
DPDPDP	1327.0	0.8348	S _β →L _β	717.0	1.5170	S _α →L _α
DRDRDR	1335.4	0.8312	S _β →L _β	718.0	1.5082	S _α →L _α
DSDSDS	1380.9	0.8408	S _β →L _β	692.2	1.2018	S _α →L _α
DSDSDA	1295.8	0.8143	S _β →L _β	705.2	1.3693	S _α →L _α
DSDADS	1438.7	0.8576	S _β →L _β	701.0	1.2591	S _α →L _α
DSDADA	1331.4	0.8208	S _β →L _β	715.6	1.4196	S _α →L _α
DADADA	1274.3	0.7980	S _β →L _β	698.2	1.3165	S _α →L _α

General Williamson Etherification Procedure

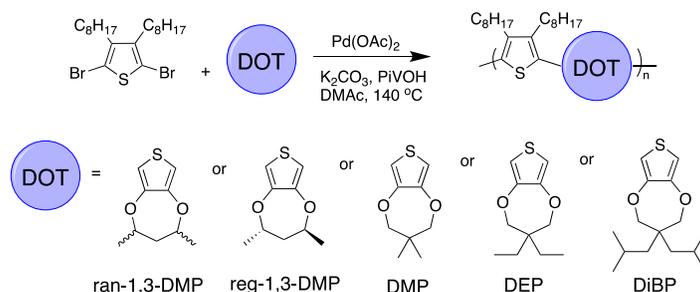


Propylenedioxythiophene comonomers were synthesized according to literature procedures. Briefly, a Soxhlet extraction apparatus consisting of a two-neck roundbottom flask, extractor, and condenser was dried overnight in a high temperature oven. The next day, the apparatus was assembled while still hot, equipped with a Teflon stir bar, a Soxhlet thimble filled with activated 4Å sieves, sealed with a rubber septum, and cooled to room temperature under a stream of argon (Ar). After the Soxhlet apparatus cooled to room temperature, 3,4-dimethoxythiophene (1.0 equiv.) and the appropriate diol (2.0 equiv.) were weighed into vials and subsequently transferred to the Soxhlet apparatus by rinsing the vials with 3 successive washes with toluene. Toluene was then added to the Soxhlet apparatus via cannula transfer to create a 0.1 M solution with respect to 3,4-dimethoxythiophene and the apparatus was placed in an oil bath set to 110 °C. After heating the solution to 110 °C, *p*-toluenesulfonic acid (10 mol. %) was added in one portion and the reaction proceeded for 24 h. After 24 h, the reaction was cooled to room temperature, extracted with dichloromethane and washed with brine (150 mL) and water (150 mL). The recovered organic

fractions were dried with MgSO_4 , filtered, and concentrated via rotary evaporation. The crude oils were subsequently purified via silica column chromatography using 15:1 (v/v) hexanes:ethyl acetate as the mobile phase. The desired propylenedioxythiophene was collected as the first fraction, concentrated via rotary evaporation, and dried under vacuum overnight.

DiisobutylProDOT: Pale yellow oil. Yield (%) = 46%, ^1H NMR: (500 MHz, CDCl_3), δ (ppm): 0.96 (d, 12 H), 1.43 (d, 4 H), 1.73-1.80 (m, 2 H), 3.93 (s, 4H), 6.41 (s, 2H). ^{13}C NMR: (500 MHz, CDCl_3), δ (ppm): 23.24, 25.22, 42.11, 45.29, 78.12, 104.23, 149.51. HR ESI MS calc'd for $\text{C}_{15}\text{H}_{24}\text{O}_2\text{S}$: 269.1570 Found: 269.1566

General Direct Arylation Polymerization Procedure



Pd(OAc)_2 (2 mol. %), PivOH (0.3 mol. equiv.), and K_2CO_3 (2.5 mol. equiv.), were added to a Schlenk flask equipped with a Teflon stir bar and was sealed with a rubber septum the atmosphere was rendered inert via 3 vacuum/refill cycles with Ar. 2,5-Bisbromo-3,4-dioctylthiophene (1.0 mol. equiv.) and the desired ProDOT (1.0 mol. equiv.) were weighed in vials and transferred to the reaction flask using degassed DMAc and the reaction flask was placed in an oil bath set to 140 $^\circ\text{C}$. The reaction was then allowed to stir for 18-21 h. After the allotted reaction time, the reaction flask was removed from the oil bath and cooled to room temperature. The reaction mixture was then precipitated into a copious amount of methanol (MeOH) and stirred for 1 h. After 1 h, the

precipitate was filtered into a Soxhlet thimble and the polymer was purified with subsequent washes with MeOH, acetone, and extracted with chloroform. The palladium scavenger diethylammonium diethylcarbamate and 18-crown-6 were added to the polymer/chloroform solution and the mixture was subsequently stirred for 2 h. After 2 h, the solution was concentrated via rotary evaporation and then the concentrated fraction was precipitated in MeOH. The precipitate was then filtered, washed with MeOH (300 mL), and dried under vacuum.

DAT-co-(reg-1,3-DMP): Orange solid. $M_n = 29.1$ kg/mol, $M_w = 69.3$ kg/mol, $D = 2.4$, Yield (%) = 92%. ^1H NMR (700 MHz, CDCl_3) δ (ppm): 4.60-4.66 (br, m), 2.7-2.8 (br, s), 2.10-2.17 (br, m), 1.50-1.62 (br, s), 1.45-1.48 (br, d), 1.39-1.44 (br, m), 1.25-1.36 (br, m), 0.86-0.92 (br, m). Anal. calcd. for $\text{C}_{31}\text{H}_{50}\text{O}_2\text{S}_2$: C 70.97, H 9.45, S 13.06 Found: C 71.11, H 9.37, S 12.98.

DAT-co-DMP: Reddish-brown solid. $M_n = 18.1$ kg/mol, $M_w = 38.0$ kg/mol, $D = 2.1$, Yield (%) = 83%. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 3.83-3.92 (br, s), 2.66-2.76 (br, s), 1.53-1.63 (br, s), 1.38-1.45 (br, s), 1.24-1.38 (br, m), 1.07-1.14 (br, s) 0.88-0.94 (br, m). Anal. calcd. for $\text{C}_{31}\text{H}_{50}\text{O}_2\text{S}_2$: C 70.97, H 9.45, S 13.06 Found: C 70.70, H 8.98, S 13.04.

DAT-co-DEP: Red solid. $M_n = 19.9$ kg/mol, $M_w = 53.8$ kg/mol, $D = 2.7$, Yield (%) = 87%. ^1H NMR (500 MHz, CDCl_3) δ (ppm): 3.94-4.02 (br, s), 2.65-2.75 (br, s), 1.47-1.62 (br, multiple peaks), 1.37-1.45 (br, s), 1.25-1.36 (br, m), 0.87-0.95 (br, m). Anal. calcd. for $\text{C}_{33}\text{H}_{54}\text{O}_2\text{S}_2$ C 71.76, H 9.71, S 12.36 Found: C 71.79, H 9.54, S 12.29.

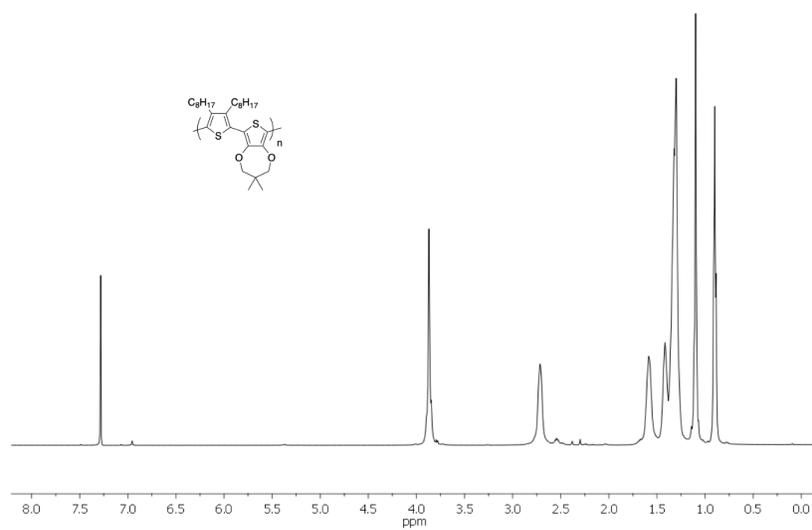


Figure S4. ^1H NMR (500 MHz, 25 °C, CDCl_3) of DAT-co-DMP.

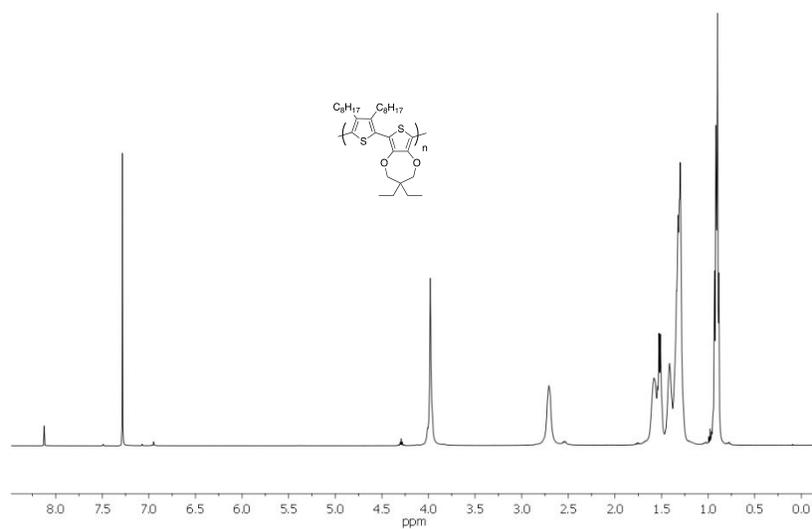


Figure S5. ^1H NMR (500 MHz, 25 °C, CDCl_3) of DAT-co-DEP.

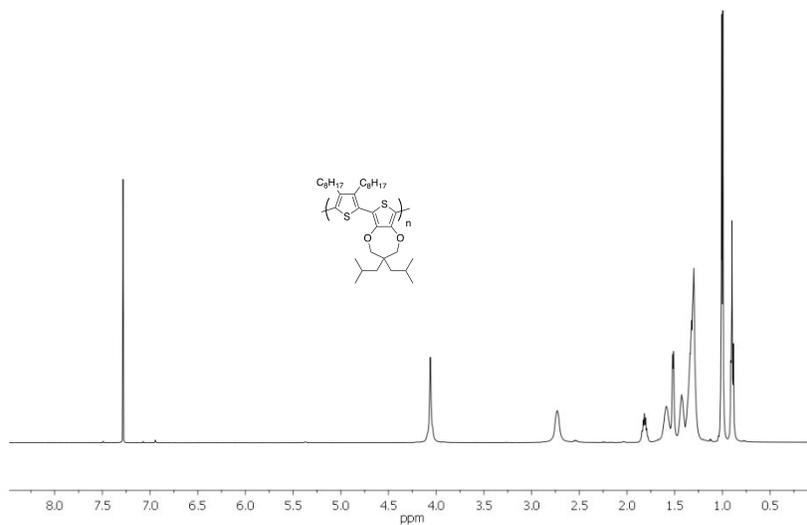


Figure S6. ¹H NMR (500 MHz, 25 °C, CDCl₃) of DAT-co-DiBP.

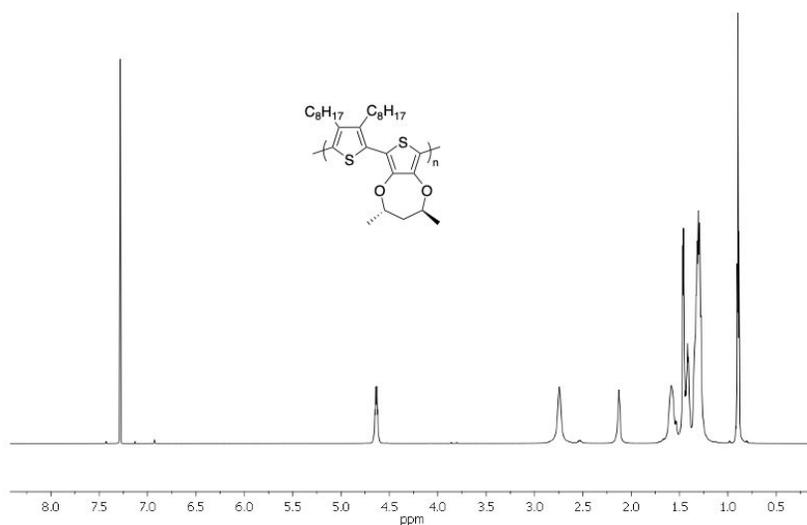


Figure S7. ¹H NMR (700 MHz, 25 °C, CDCl₃) of DAT-co-(reg-1,3-DMP).

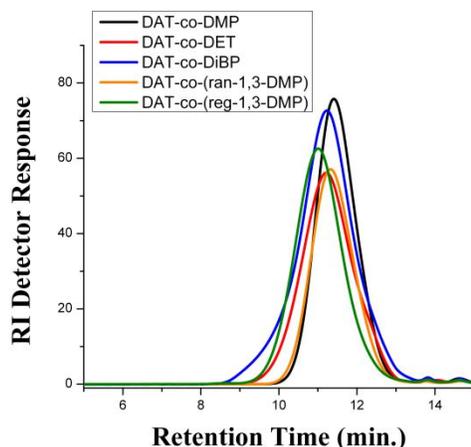


Figure S8. SEC elugrams for DAT-ProDOT copolymers while using CHCl_3 as the eluent at $35\text{ }^\circ\text{C}$ with a flow rate of 1 mL/min .

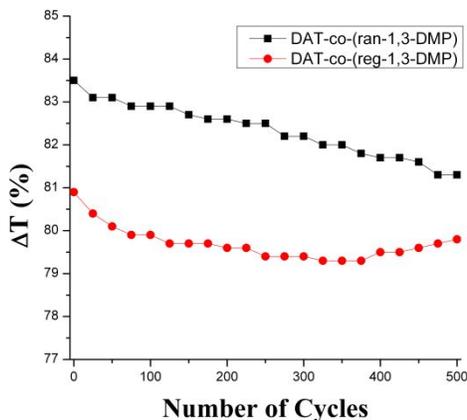


Figure S9. Contrast ($\Delta T(\%)$) as a function of the number of redox switching cycles while applying square-wave potentials between -0.5 V to 0.6 V vs Ag/Ag^+ in a $0.5\text{ M TBAPF}_6/\text{PC}$ electrolyte solution in an inert argon environment.

$$\Delta E_{ab}^* = \sqrt{(\Delta L^*)^2 + (\Delta a^*)^2 + (\Delta b^*)^2} \quad \text{Eq. S1}$$

Table S5. Quantitative color change of stereorandom and stereospecific copolymers between electrochemically conditioned films and the same film after 500 switching cycles.

Polymer	ΔE_{ab}^*
DAT-co-(ran-1,3-DMP)	1.5
DAT-co-(reg-1,3-DMP)	9.0



Figure S10. Photograph of films consisting of (left) DAT-co-(reg-1,3-DMP) and (right) DAT-co-(ran-1,3-DMP) after 500 redox switching cycles.

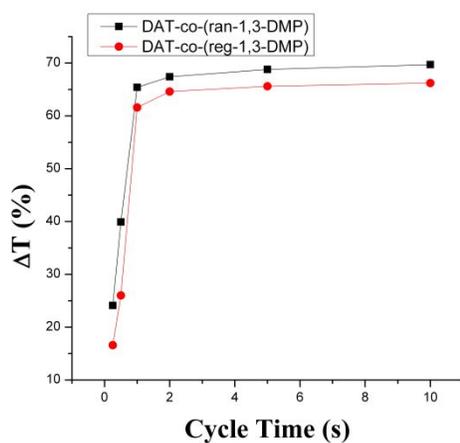


Figure S11. Transmittance at λ_{\max} as a function of switching time.

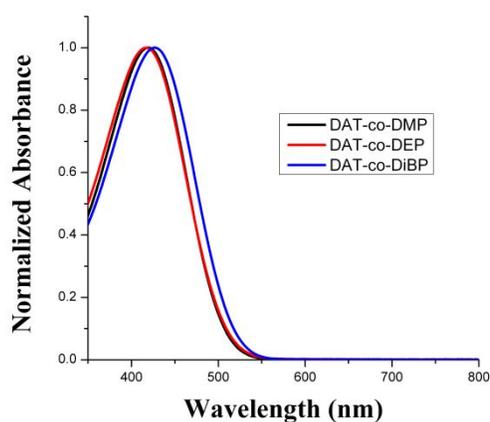


Figure S12. Normalized solution UV-vis absorbance spectra of DAT-co-(2,2-ProDOTs) dissolved in toluene with nominal concentrations of $15 \mu\text{g/mL}$.

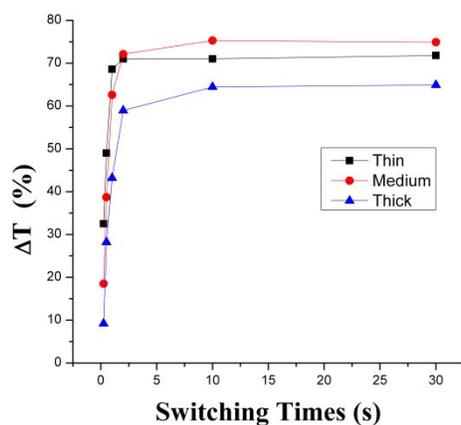


Figure S13. Transmittance at λ_{\max} as a function of switching time for DAT-co-ProDOT films of varying thickness.

Table S6. Quantitative color change of 2,2-substituted copolymers^a.

Polymer	ΔE_{ab}^*
DAT-DMP	17.4
DAT-DEP	6.7
DAT-DiBP	1.8

^aQuantitative color change calculated between electrochemically conditioned films and the film after 500 electrochemical switching cycles.

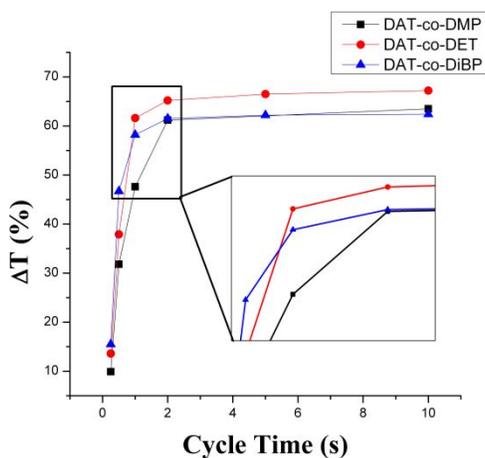


Figure S14. Transmittance at λ_{\max} as a function of switching time of 2,2-substituted DAT-ProDOT copolymers.

Optimized Coordinates from Computation

A. DPDPDP

a. Neutral

C	-0.78924300	0.82922000	-0.18547800
C	-1.45008500	1.99728200	-0.55433200
C	-2.85838400	1.80871700	-0.74201500
C	-3.26825000	0.50189000	-0.49668500
S	-1.91066700	-0.50410000	-0.06034200
C	-4.58793200	-0.09828700	-0.52407200
C	-4.90555500	-1.44553500	-0.56841100
S	-6.06556600	0.83372900	-0.45368800
C	-6.30531900	-1.71135800	-0.54409700
C	-7.09461900	-0.57761600	-0.45617800
C	-0.78636900	3.34037500	-0.71085500
H	0.12281100	3.24672800	-1.32449100
H	-1.44721900	4.00126400	-1.28825100
C	-3.77198000	2.91461500	-1.19952000
H	-3.24463000	3.52106100	-1.95211500
H	-4.62807300	2.47877200	-1.73496500
C	-4.27876500	3.82958000	-0.08352800
H	-4.82077900	3.26086100	0.68648200
H	-3.45040900	4.35392300	0.41363400
H	-4.96345200	4.58995000	-0.48760100
C	-0.44455700	4.01619700	0.61917200
H	0.02452800	4.99619500	0.44664000
H	-1.34758400	4.17366400	1.22668200
H	0.25329300	3.40807600	1.21241200
O	-3.95612700	-2.40634900	-0.69347600
O	-6.83998300	-2.95026600	-0.68786800
C	-3.96495600	-3.44339500	0.29682200
C	-6.46261800	-3.92384600	0.29466600
C	-5.06384200	-4.46256600	0.07500000
H	-4.04112500	-2.98860000	1.29946000
H	-6.56709300	-3.48467600	1.30154700
H	-2.97894700	-3.91681400	0.20822000
H	-7.20406200	-4.72588200	0.19043700
C	0.61955100	0.56858500	0.03741400
S	1.89335700	1.65786000	-0.46388900
C	1.19109000	-0.56503200	0.59165600
C	3.17270900	0.62375500	0.12867400
C	2.61325700	-0.53376500	0.64219600
O	0.45084600	-1.63388300	0.97843400
C	4.58238700	0.94400400	0.00889000
O	3.37227100	-1.56863600	1.08136000
C	0.60165600	-2.04872200	2.34326000

C	5.21823400	2.13792500	-0.32138000
S	5.75417100	-0.33110000	0.24961400
C	3.14589400	-1.99237100	2.43311400
C	1.88467700	-2.81867700	2.58240400
H	0.53664600	-1.16511700	3.00069900
H	-0.26932600	-2.68701800	2.53761800
C	6.64524700	2.00873400	-0.40053000
C	4.51709100	3.45072300	-0.55271400
C	7.08185700	0.72621700	-0.11765600
H	3.12601800	-1.10773000	3.09211100
H	4.02886900	-2.59167500	2.68806200
C	7.56840500	3.12426100	-0.81300900
H	5.19810300	4.12456800	-1.09136300
H	3.66102800	3.31299700	-1.23122300
C	4.05034700	4.13423200	0.73468300
H	8.50980300	2.68205300	-1.17069100
H	7.13297200	3.64446700	-1.68169500
C	7.87843700	4.14563200	0.28142100
H	3.33358400	3.50814700	1.28514200
H	4.89826400	4.33669400	1.40506300
H	3.55837500	5.09206300	0.50925600
H	8.58878200	4.90043300	-0.08730300
H	6.97431900	4.67371100	0.61622100
H	8.32588800	3.66331900	1.16320900
C	8.43187500	0.18430300	-0.07078900
S	9.73104700	0.99441200	0.76731600
C	8.88544000	-1.00399000	-0.61069400
C	10.85246400	-0.25920700	0.39903700
C	10.27527000	-1.25201600	-0.34546800
O	8.09656000	-1.78424900	-1.39108900
O	10.98932700	-2.29486500	-0.84351100
C	8.01047400	-3.16480500	-1.02431500
C	10.47838200	-3.59954900	-0.55754800
C	9.25364300	-3.95733700	-1.37659700
H	7.78527100	-3.24388800	0.05381900
H	7.14507400	-3.54443500	-1.58227900
H	10.26802700	-3.68206400	0.52351000
H	11.30631700	-4.27935900	-0.79640800
C	-8.54475200	-0.50286300	-0.45804600
C	-9.39685100	0.55366000	-0.14950900
S	-9.46108400	-1.91098900	-0.95849600
C	-10.78226600	0.21714000	-0.33965000
C	-8.96015100	1.90159800	0.36192400
C	-10.94742900	-1.07271900	-0.77253000
C	-11.94657800	1.14135400	-0.10065400
H	-8.15354200	2.30853600	-0.26760600

H	-9.79490500	2.60724400	0.24336000
C	-8.51599700	1.89485600	1.82645200
H	-11.88462400	-1.58189100	-0.98896800
H	-11.71944900	2.13915200	-0.51009700
H	-12.80490000	0.76800000	-0.67941600
C	-12.35351500	1.27180400	1.36668600
H	-8.22891400	2.90665900	2.14922800
H	-9.32512800	1.54512600	2.48409400
H	-7.65143400	1.23364200	1.98168900
H	-12.61006200	0.28953500	1.79110300
H	-11.54541900	1.69876600	1.97817800
H	-13.23153000	1.92678200	1.46962100
H	11.89074500	-0.19367900	0.71211700
H	9.47827200	-3.83310000	-2.44786800
H	9.03368800	-5.02511100	-1.21193200
H	1.85732100	-3.21892400	3.60928800
H	-4.90351600	-5.29630400	0.77821700
H	1.92802000	-3.68057100	1.89801900
H	-4.98341700	-4.87459100	-0.94318500

b. Radical Cation

C	-10.89927000	-0.06244400	-0.30940500
C	-10.23832400	1.12643100	-0.14849400
S	-9.82371900	-1.39272400	-0.44706600
C	-8.81973300	0.95232800	-0.11271900
C	-8.41204500	-0.37468100	-0.24276200
O	-10.88491500	2.31658100	-0.12324000
O	-7.92430500	1.96023100	-0.04387700
C	-10.58973600	3.17990400	0.97946000
C	-8.06257700	2.88633300	1.04694400
C	-9.22823700	3.83652200	0.87412500
H	-10.68602500	2.61457900	1.92279800
H	-8.14419000	2.31970100	1.98967900
H	-9.14193600	4.35629600	-0.09295300
H	-9.15613800	4.60271800	1.66331300
H	-11.38133900	3.93894700	0.95326400
H	-7.11406600	3.43673700	1.05514100
C	-7.05415000	-0.86164000	-0.27025900
C	-6.56440900	-2.17918700	-0.28111500
S	-5.75554400	0.29598100	-0.34605200
C	-5.15162500	-2.24177500	-0.36312500
C	-7.43091800	-3.40466800	-0.17353300
C	-4.54395400	-0.96990900	-0.38717100
C	-4.40020000	-3.54170900	-0.43616700
H	-8.29251400	-3.31749300	-0.85224700
H	-6.87109000	-4.27377400	-0.54322900
C	-7.91292300	-3.69452000	1.25059300

C	-3.16576300	-0.60761200	-0.41862600
H	-5.01204300	-4.27219800	-0.98413800
H	-3.50234100	-3.41339000	-1.05777400
C	-4.01738500	-4.12794200	0.92486000
H	-8.53782000	-4.59915100	1.26605500
H	-7.06431500	-3.85587800	1.93039900
H	-8.51046700	-2.86525300	1.65493800
C	-2.63870300	0.69577100	-0.51158900
S	-1.85436200	-1.76087800	-0.35085600
H	-3.40678700	-3.42667700	1.51187600
H	-4.90998100	-4.37027900	1.51795600
H	-3.43855300	-5.05318600	0.79226400
C	-1.23701700	0.74403700	-0.50545000
O	-3.45901800	1.74971700	-0.68635200
C	-0.61869800	-0.52118400	-0.40877600
O	-0.49000700	1.85010800	-0.66549100
C	-3.28559500	2.89581600	0.16357500
C	-0.75657900	2.98632600	0.17598200
C	-2.04622000	3.69342800	-0.17333700
H	-3.27500900	2.56487800	1.21542400
H	-4.19007000	3.49175400	-0.00527500
H	-0.75286300	2.65835300	1.22862400
H	0.10474400	3.64385400	0.01159700
H	-2.05112100	3.96260700	-1.24078800
H	-2.08060100	4.63308200	0.40111600
C	0.77509300	-0.78224400	-0.36590400
C	1.47241200	-2.01712600	-0.33112500
S	1.89565500	0.56502000	-0.34023100
C	2.86864500	-1.86059600	-0.25673600
C	0.80308900	-3.36196300	-0.38327200
C	3.27527600	-0.50365600	-0.25434300
C	3.81840600	-3.02124100	-0.15166000
H	-0.08799900	-3.30255300	-1.02476900
H	1.46773700	-4.06824400	-0.89955500
C	0.42848700	-3.93517500	0.98585300
C	4.58381900	0.06286800	-0.22751200
H	3.33277900	-3.92054500	-0.55235100
H	4.68495700	-2.85631300	-0.80919300
C	4.28844300	-3.30476800	1.27814800
H	-0.09593500	-4.89377700	0.86538400
H	1.32215900	-4.11372900	1.59930200
H	-0.23057000	-3.25614000	1.54565700
C	4.90754500	1.42638600	-0.16073000
S	6.06449600	-0.86913900	-0.32275400
H	4.79801100	-2.43685400	1.71999600
H	3.44136200	-3.56033900	1.92977800

H	4.99148800	-4.14991400	1.28684700
C	6.29379400	1.68892500	-0.16208100
O	3.94622100	2.36820000	-0.16376300
C	7.08596400	0.54006800	-0.22598800
O	6.84493100	2.92205400	-0.19501800
C	3.98536500	3.36768100	0.87251200
C	6.47857000	3.83558600	0.85060100
C	5.08205400	4.38985700	0.67096000
H	4.08132900	2.86317100	1.84801800
H	2.99854900	3.84213400	0.82208900
H	6.58907400	3.33290800	1.82603000
H	7.22469300	4.63648400	0.78659800
H	4.98840500	4.84633700	-0.32656100
H	4.93416300	5.19174200	1.41236800
C	8.52463800	0.47966500	-0.27120300
C	9.38813900	-0.62257000	-0.26469300
S	9.43437600	1.97780200	-0.38884300
C	10.76397700	-0.23997000	-0.37202700
C	8.96524900	-2.05996500	-0.13352100
C	10.91513900	1.12405900	-0.44256100
C	11.94065600	-1.17766300	-0.41537700
H	8.10891000	-2.26812500	-0.79371900
H	9.77644700	-2.69725000	-0.51303900
C	8.63235100	-2.47953700	1.30140100
H	11.84852500	1.67644500	-0.53523700
H	11.69425200	-2.05596900	-1.03260700
H	12.76387200	-0.66655100	-0.93667500
C	12.42938900	-1.63588600	0.95826800
H	8.34447500	-3.54042200	1.33386500
H	9.49787100	-2.34159700	1.96467200
H	7.80084800	-1.89130200	1.71511500
H	12.70402900	-0.77438300	1.58510400
H	11.66029000	-2.20911800	1.49542200
H	13.31564600	-2.27941800	0.85730300
H	-11.97321300	-0.20917500	-0.38525800

B. DRDRDR

a. Neutral

C	1.00351400	-1.33857400	-0.16771600
C	1.69910300	-2.52290200	-0.38811300
C	3.10363000	-2.31744500	-0.58485600
C	3.47450500	-0.97952600	-0.49411800
S	2.08503400	0.03124300	-0.19138700
C	4.77728600	-0.34928700	-0.57999800
C	5.05792000	0.99019500	-0.78979000
S	6.28060500	-1.21876100	-0.37054200
C	6.44721500	1.29973900	-0.78276700

C	7.26745400	0.21257500	-0.53983100
C	1.07259800	-3.89310600	-0.37806100
H	0.18222500	-3.91108000	-1.02513000
H	1.76823800	-4.60926000	-0.83631900
C	4.05339400	-3.44283400	-0.89735500
H	3.55601400	-4.14444900	-1.58501800
H	4.90907300	-3.04743600	-1.46393000
C	4.55910800	-4.21109400	0.32459800
H	5.06855400	-3.54361900	1.03533200
H	3.73405900	-4.69993700	0.86224600
H	5.27250000	-4.99208900	0.02244100
C	0.70075200	-4.38490800	1.02250300
H	0.26190100	-5.39260800	0.97579600
H	1.58568600	-4.42934700	1.67420000
H	-0.03236300	-3.71950600	1.50076400
O	4.08911900	1.90403600	-1.04642400
O	6.93975100	2.52864000	-1.07892300
C	4.05980100	3.05583600	-0.19569700
C	6.51740700	3.60193300	-0.23114500
C	5.10876900	4.11775100	-0.53443000
H	4.15796600	2.73496200	0.85575400
H	6.59817100	3.28673100	0.82333600
H	3.05306000	3.47322500	-0.33547800
H	7.25039900	4.40043900	-0.40968000
C	4.85504300	5.31665700	0.38402800
H	5.58789700	6.11423200	0.19256800
H	3.85193300	5.73351200	0.21079000
H	4.92712800	5.03820000	1.44681900
C	4.99636300	4.53186500	-2.00161600
H	3.99098000	4.92339700	-2.21820700
H	5.72624200	5.32070300	-2.23844900
H	5.18327000	3.68079600	-2.66919100
C	-0.41458900	-1.09203400	0.00646700
S	-1.65606200	-2.22322100	-0.48225700
C	-1.01965500	0.05648500	0.48723000
C	-2.96961800	-1.18240000	0.02077200
C	-2.44036000	0.00484200	0.49803300
O	-0.31457800	1.15876700	0.84365200
C	-4.36967100	-1.52690100	-0.13369000
O	-3.21714300	1.05206900	0.87126300
C	-0.51074400	1.62926400	2.18232100
C	-4.98074100	-2.74302100	-0.42317300
S	-5.55494700	-0.24819300	-0.03141900
C	-3.02865100	1.53476700	2.20678300
C	-1.79971700	2.43105800	2.37910400
H	-0.47202900	0.77304300	2.87726400

H	0.35753800	2.27279500	2.37942600
C	-6.40306100	-2.63365200	-0.57055900
C	-4.25431100	-4.05736000	-0.54067300
C	-6.86907100	-1.33947200	-0.37475500
H	-2.98770000	0.67764900	2.90048600
H	-3.93873300	2.11061700	2.42353100
C	-1.80530200	2.93968000	3.82360300
C	-1.85249300	3.60236900	1.39790500
C	-7.27703900	-3.80021900	-0.94736300
H	-4.90121100	-4.77882100	-1.05855100
H	-3.37425300	-3.94947800	-1.19332700
C	-3.82845700	-4.64714200	0.80605600
H	-0.93744700	3.58938700	4.00973900
H	-2.71330800	3.52711300	4.02456700
H	-1.77014100	2.11140600	4.54806100
H	-2.76606400	4.19604500	1.55269100
H	-0.98732600	4.26720500	1.54151700
H	-1.84462200	3.24962700	0.35842000
H	-8.18025600	-3.42441300	-1.44976700
H	-6.75440600	-4.40373500	-1.70589100
C	-7.68262400	-4.70191200	0.21953600
H	-3.14152900	-3.97542200	1.34053700
H	-4.69881400	-4.81902100	1.45595300
H	-3.31567100	-5.60985800	0.66281100
H	-8.34997400	-5.50495700	-0.12680700
H	-6.80753900	-5.17253400	0.68983400
H	-8.21249100	-4.13507100	0.99939200
C	-8.22076800	-0.80572300	-0.38589400
S	-9.63843200	-1.78363500	-0.07640100
C	-8.60970400	0.50738300	-0.59464800
C	-10.70470500	-0.43926000	-0.21776100
C	-10.02421600	0.71103700	-0.50740900
O	-7.72729600	1.48213800	-0.92988500
O	-10.64603200	1.89034800	-0.76629800
C	-7.73533200	2.65224400	-0.10647700
C	-10.22935200	3.00306100	0.02684900
C	-8.88939400	3.61789700	-0.38886500
H	-7.73308100	2.35172500	0.95574900
H	-6.77864300	3.14663300	-0.32499800
H	-10.20401200	2.70591900	1.09022000
H	-11.02790700	3.74712400	-0.10107000
C	-8.66801700	4.85611100	0.48468600
C	-8.91458800	4.00140000	-1.86835200
H	-7.71393700	5.34344200	0.23508300
H	-9.47133100	5.59107300	0.32819100
H	-8.64725000	4.60005900	1.55541000

H	-9.72322800	4.72059300	-2.06858800
H	-7.96344700	4.46910000	-2.16461300
H	-9.07524800	3.12052000	-2.50347800
C	8.71915300	0.18121300	-0.51681700
C	9.59479300	-0.76716400	0.00226200
S	9.60093600	1.48676800	-1.28223600
C	10.97252900	-0.43471000	-0.24200400
C	9.18416800	-1.99337700	0.77612700
C	11.10764500	0.74651100	-0.92451400
C	12.15823100	-1.25437100	0.19189000
H	8.41229000	-2.55458600	0.22684900
H	10.04374300	-2.67653200	0.83277400
C	8.68863700	-1.69181000	2.19205500
H	12.03306100	1.23081700	-1.23025500
H	11.96468400	-2.32148000	-0.00401600
H	13.01501200	-0.98311700	-0.44325400
C	12.54379600	-1.06566200	1.65867700
H	8.42267500	-2.62166700	2.71640300
H	9.46218700	-1.17833400	2.78179100
H	7.79821300	-1.04687000	2.17647500
H	12.77367700	-0.01069100	1.87091600
H	11.73344700	-1.37297300	2.33560200
H	13.43264900	-1.66431300	1.90787000
H	-11.77900600	-0.56611500	-0.11903600

b. Radical Cation

C	1.00144800	-1.24547100	-0.21904500
C	1.71719700	-2.46750700	-0.14008500
C	3.11277100	-2.29243800	-0.17077700
C	3.49901500	-0.93167000	-0.25250500
S	2.10096100	0.11489300	-0.31749700
C	4.79803500	-0.34589500	-0.29570000
C	5.10054400	1.02015000	-0.39982400
S	6.29612500	-1.25414100	-0.23284100
C	6.48050600	1.30507300	-0.41502100
C	7.29288000	0.17431200	-0.30806500
C	1.06408900	-3.81288600	0.00717300
H	0.20597800	-3.88964800	-0.67719600
H	1.76072600	-4.59034000	-0.33177500
C	4.08419600	-3.43923800	-0.12317700
H	3.61917400	-4.31936800	-0.58774400
H	4.94784100	-3.21450500	-0.76566200
C	4.55762100	-3.80540400	1.28534100
H	5.02528100	-2.94923600	1.79226300
H	3.72017000	-4.14663800	1.90948000
H	5.29745700	-4.61729900	1.23931100
C	0.62578900	-4.12799300	1.44054400

H	0.14258700	-5.11452500	1.48162400
H	1.48727000	-4.14215900	2.12239400
H	-0.08897200	-3.38505300	1.82192800
O	4.13019700	1.94041000	-0.54547600
O	7.00487200	2.53346600	-0.61427700
C	4.14355200	3.07501600	0.33927100
C	6.60370800	3.57493800	0.28629200
C	5.20431300	4.12491000	0.01028300
H	4.25499900	2.71531600	1.37549700
H	6.68365400	3.20847500	1.32345400
H	3.14154200	3.50827900	0.22591700
H	7.35227900	4.36394300	0.13779800
C	4.98236400	5.30059200	0.96750600
H	5.72481800	6.09105900	0.78568300
H	3.98371400	5.73727300	0.82102600
H	5.06700800	4.99136400	2.02060700
C	5.07999600	4.58272400	-1.44286500
H	4.08054900	5.00198600	-1.63198800
H	5.82308400	5.36255200	-1.66645200
H	5.23925800	3.74992700	-2.14014500
C	-0.39617700	-1.00623800	-0.25701200
S	-1.61127200	-2.26629100	-0.33312000
C	-1.03688800	0.25021800	-0.28158500
C	-2.94276500	-1.13284100	-0.35945400
C	-2.43437400	0.18002600	-0.33179400
O	-0.32210600	1.38769100	-0.32981500
C	-4.31434100	-1.51673900	-0.40878100
O	-3.25427400	1.24361700	-0.43612500
C	-0.62397300	2.41643100	0.62951200
C	-4.90073000	-2.79574900	-0.49199100
S	-5.54688900	-0.27181100	-0.35373900
C	-3.12638500	2.28583900	0.54341500
C	-1.91005000	3.18856000	0.34074900
H	-0.65332400	1.96634400	1.63566100
H	0.24014200	3.09042800	0.57358100
C	-6.31674900	-2.75729600	-0.48002100
C	-4.12291800	-4.07761900	-0.60000000
C	-6.82840700	-1.44962600	-0.41342700
H	-3.11626200	1.83375300	1.54916600
H	-4.04925200	2.86935200	0.43220200
C	-2.00396700	4.31097600	1.37971000
C	-1.89152700	3.76593500	-1.07464900
C	-7.16795200	-3.99776400	-0.50035000
H	-4.69958700	-4.79137500	-1.20488100
H	-3.20546100	-3.90328900	-1.18064700
C	-3.77884000	-4.72265800	0.74469800

H	-1.14782400	4.99530400	1.29034600
H	-2.92088600	4.89881800	1.22901100
H	-2.01807600	3.91693100	2.40739400
H	-2.80511900	4.34839100	-1.26514900
H	-1.02847700	4.43513100	-1.20746100
H	-1.82851900	2.97341200	-1.83166800
H	-8.00385800	-3.86703500	-1.20384300
H	-6.58232900	-4.82875200	-0.91515000
C	-7.70012400	-4.40441100	0.87650400
H	-3.20158200	-4.04138200	1.38637800
H	-4.68780200	-5.00693600	1.29249900
H	-3.17987000	-5.63139700	0.58916800
H	-8.31783000	-5.31043500	0.79515300
H	-6.87648600	-4.61628900	1.57281500
H	-8.31898000	-3.61361400	1.32369800
C	-8.19368100	-0.98365900	-0.42074500
S	-9.58351800	-2.01413100	-0.70340200
C	-8.62796600	0.33142500	-0.26084400
C	-10.68386900	-0.70413500	-0.56380200
C	-10.04472800	0.48672600	-0.34260900
O	-7.75833200	1.35457700	-0.12597500
O	-10.70068000	1.67088200	-0.30558700
C	-7.95726800	2.23983200	0.98757000
C	-10.45721200	2.50053600	0.83277700
C	-9.11066600	3.22837900	0.81216900
H	-8.09243300	1.63927300	1.90275000
H	-7.00830700	2.78607500	1.06819800
H	-10.55838900	1.89914700	1.75312300
H	-11.27235300	3.23643800	0.81283800
C	-9.08442700	4.16657200	2.02322900
C	-8.94758800	4.02102200	-0.48475100
H	-8.13362300	4.71750600	2.06841000
H	-9.89733900	4.90431900	1.95774500
H	-9.20262800	3.61515300	2.96878100
H	-9.75642500	4.75946000	-0.59038600
H	-7.99027100	4.56359800	-0.48997800
H	-8.97194800	3.36103400	-1.36162200
C	8.73263500	0.13398800	-0.32447200
C	9.61295500	-0.93353500	-0.11214500
S	9.61903000	1.60171400	-0.70457800
C	10.98332900	-0.55310500	-0.27884800
C	9.21094000	-2.32799200	0.28329400
C	11.11365000	0.77758300	-0.59655200
C	12.17407600	-1.46320700	-0.13806000
H	8.37896800	-2.67986800	-0.34639000
H	10.04432200	-3.00741800	0.05610000

C	8.84129500	-2.46901000	1.76259000
H	12.03920600	1.31995000	-0.78114100
H	11.94647100	-2.44492100	-0.58266200
H	12.99570500	-1.04488500	-0.73850900
C	12.65234000	-1.64942400	1.30141200
H	8.57034800	-3.50964600	1.99281700
H	9.68381500	-2.18577700	2.40926600
H	7.98741800	-1.83051300	2.03062100
H	12.91049100	-0.68217900	1.75783200
H	11.88302600	-2.12095800	1.92959600
H	13.54651700	-2.28924700	1.33148300
H	-11.75203100	-0.86369600	-0.68281200

C. DSDSDS

a. Neutral

C	-1.03697900	0.99910300	0.05304500
C	-1.62196400	2.16923100	0.51342600
C	-3.05079000	2.15708100	0.39634000
C	-3.54434200	0.96741200	-0.13622200
S	-2.23552900	-0.12034200	-0.52070300
C	-4.90636200	0.52536600	-0.37308400
C	-5.32811100	-0.59676400	-1.07170200
S	-6.30794500	1.38516500	0.22496500
C	-6.74680500	-0.75511800	-1.11215400
C	-7.43183800	0.22200400	-0.42089500
C	-0.84864000	3.30686100	1.13165500
H	-0.05505700	3.64421300	0.44784300
H	-1.51206200	4.17380900	1.25199700
C	-3.89775900	3.33106000	0.80823500
H	-3.36369500	4.25873300	0.55172900
H	-4.81400700	3.35774700	0.20079400
C	-4.26038800	3.35339700	2.29394400
H	-4.80976500	2.44590000	2.58500700
H	-3.36056600	3.41309400	2.92367000
H	-4.89334200	4.22251000	2.52693900
C	-0.23247900	2.95368600	2.48588200
H	0.30482000	3.81737800	2.90486200
H	-1.00618600	2.65149500	3.20739300
H	0.48201400	2.12270700	2.39371300
O	-4.46325500	-1.42083600	-1.71434300
O	-7.38034800	-1.72268400	-1.81768100
C	-4.51580200	-2.82728600	-1.37321400
C	-7.07783000	-3.08570000	-1.45158000
C	-5.72396000	-3.51134300	-1.99512800
H	-4.57085900	-2.90134000	-0.27227900
H	-7.07129600	-3.14446300	-0.34815700
H	-5.70708100	-3.35271000	-3.08608000

H	-5.61653900	-4.59403800	-1.82169700
C	-3.21508400	-3.42409500	-1.86841400
H	-3.13153300	-3.30634800	-2.95890500
H	-2.35319300	-2.93625500	-1.39649500
H	-3.18032000	-4.49672400	-1.63342800
C	-8.21278200	-3.92210900	-2.00256100
H	-8.08189100	-4.97628700	-1.72287800
H	-9.17474900	-3.57103600	-1.60650000
H	-8.24197500	-3.85501700	-3.10019000
C	0.36462600	0.63649600	-0.06592600
S	1.57511100	1.78824500	-0.56566000
C	0.94092400	-0.61301400	0.05970100
C	2.86765500	0.60981900	-0.54301200
C	2.34554400	-0.62585900	-0.18942800
O	0.21496900	-1.72625800	0.32640200
C	4.24685500	0.93736300	-0.85257300
O	3.10190200	-1.75151700	-0.15675400
C	0.58195900	-2.45583100	1.51846700
C	4.82037100	2.11293700	-1.33446200
S	5.47435700	-0.27473500	-0.58425300
C	3.12162300	-2.49312600	1.08711400
C	1.83672500	-3.28175000	1.28865700
H	0.76311600	-1.71770800	2.32039300
C	-0.61454300	-3.31237700	1.87322400
C	6.24769600	2.03319100	-1.45327900
C	4.05611000	3.35500900	-1.70634300
C	6.74578700	0.79592900	-1.08169900
H	3.24347800	-1.76393500	1.90803000
C	4.33267800	-3.39940500	1.01618600
H	1.67844200	-3.94396700	0.42146100
H	1.97994100	-3.92770800	2.16958900
H	-0.42400000	-3.86262200	2.80476900
H	-1.50751600	-2.68921200	2.01205600
H	-0.81710200	-4.04236100	1.07565900
C	7.11844700	3.18973800	-1.87592300
H	4.54092600	3.81910400	-2.57864800
H	3.05045600	3.08237200	-2.05790100
C	3.95099000	4.38659700	-0.58186000
H	4.24388600	-4.09107400	0.16544600
H	5.25455200	-2.81642200	0.89897500
H	4.41104300	-3.99328600	1.93712200
H	7.77640200	2.88516000	-2.70363700
H	6.48821000	3.99067700	-2.28535100
C	7.97111700	3.75131300	-0.73760200
H	3.44941200	3.96548100	0.30200800
H	4.94575700	4.73331000	-0.26563300

H	3.37637900	5.26482000	-0.91175400
H	8.57290300	4.60337500	-1.08710800
H	7.34295500	4.09797300	0.09662000
H	8.65980300	2.98936600	-0.34385900
C	8.11061700	0.28958600	-1.10609700
S	9.17020500	0.55062600	-2.47096100
C	8.73527700	-0.52112800	-0.17759800
C	10.44854200	-0.35347000	-1.75126800
C	10.07457700	-0.88102000	-0.54612600
O	8.10882600	-0.97831200	0.93506500
O	10.86952500	-1.71345600	0.17253600
C	8.74283000	-0.67005800	2.19579900
C	11.14817400	-1.31528500	1.52991000
C	9.95503000	-1.55588100	2.44328000
H	9.05800700	0.38861600	2.16185800
C	7.67476600	-0.85077000	3.25351800
H	11.39547900	-0.23780100	1.52220500
C	12.36404100	-2.11429800	1.94895800
H	9.65039500	-2.61307800	2.36943200
H	10.28722800	-1.38423800	3.47973100
H	8.06983800	-0.58273700	4.24291400
H	6.80768200	-0.21236000	3.03931000
H	7.33886400	-1.89779700	3.28713600
H	12.13687800	-3.19070000	1.94553600
H	13.19817900	-1.93270600	1.25815200
H	12.68061200	-1.82986700	2.96164500
C	-8.87060100	0.40142400	-0.29157200
C	-9.62225100	0.74453700	0.82138000
S	-9.87772800	0.23661300	-1.70544900
C	-11.02178900	0.87553300	0.51499600
C	-9.05308400	0.91279100	2.20745700
C	-11.28842300	0.63018300	-0.80855700
C	-12.09975800	1.21386300	1.50929200
H	-8.22921000	1.64249700	2.19275000
H	-9.82204400	1.35340000	2.85790200
C	-8.55288000	-0.39427300	2.82333100
H	-12.25806900	0.64999300	-1.30219800
H	-11.76231800	2.04051300	2.15540900
H	-12.97202300	1.59804900	0.95921800
C	-12.53291600	0.03160800	2.37559800
H	-8.16616200	-0.22308100	3.83890300
H	-9.35982300	-1.13955800	2.88754400
H	-7.74256100	-0.83051100	2.22092600
H	-12.91247700	-0.79225500	1.75270000
H	-11.69772500	-0.36094000	2.97412700
H	-13.33215100	0.32933700	3.07063700

H	11.40235800	-0.47510800	-2.25696100
b. Radical Cation			
C	-1.04109300	1.05035200	-0.20200000
C	-1.70191300	2.29914300	-0.08775600
C	-3.10215400	2.18983100	-0.15965900
C	-3.54442600	0.85418000	-0.33041300
S	-2.19322200	-0.24747300	-0.40214600
C	-4.86658200	0.33221100	-0.42017700
C	-5.24927200	-0.93837100	-0.88469200
S	-6.28745700	1.22622900	0.07140700
C	-6.64142300	-1.16541400	-0.82333100
C	-7.36632100	-0.09033800	-0.29518400
C	-0.99635400	3.60479400	0.15173100
H	-0.17625800	3.73156900	-0.57081900
H	-1.68956400	4.42810500	-0.06284800
C	-4.01815700	3.38184900	-0.11073700
H	-3.53743000	4.21451900	-0.64484400
H	-4.92742500	3.16500800	-0.68887400
C	-4.39342200	3.83764000	1.30106100
H	-4.87003100	3.03020600	1.87577900
H	-3.50904100	4.16843400	1.86333900
H	-5.09724600	4.68082500	1.25334100
C	-0.46657800	3.75885000	1.58045100
H	0.02798300	4.73352700	1.69799600
H	-1.28459100	3.70067400	2.31242300
H	0.26355500	2.97692500	1.83253300
O	-4.33929700	-1.76080800	-1.43203800
O	-7.27580000	-2.25276600	-1.30510500
C	-4.29719200	-3.16396500	-1.05807300
C	-6.82757100	-3.55509700	-0.85593200
C	-5.52023100	-3.92881600	-1.52944500
H	-4.23438700	-3.20507900	0.04338000
H	-6.68852100	-3.50016700	0.23810300
H	-5.63014500	-3.81925500	-2.62056300
H	-5.32915200	-4.99434100	-1.32748700
C	-3.02449600	-3.69756000	-1.67883900
H	-3.08350700	-3.64655200	-2.77569800
H	-2.15247900	-3.12050900	-1.34811500
H	-2.87910700	-4.74652900	-1.38794400
C	-7.94539200	-4.51877000	-1.18815900
H	-7.67972100	-5.52935500	-0.84993800
H	-8.87730400	-4.21973400	-0.69220200
H	-8.11795800	-4.55008500	-2.27375800
C	0.34734000	0.75393800	-0.23749200
S	1.58133000	1.95223200	-0.55572700
C	0.95031600	-0.51277600	-0.10959500

C	2.87815500	0.78463500	-0.49455000
C	2.34844600	-0.49579700	-0.24608000
O	0.21103000	-1.61740600	0.08993800
C	4.25053700	1.12414900	-0.70311700
O	3.13796100	-1.58786400	-0.24925400
C	0.55846000	-2.44110800	1.23907300
C	4.84865100	2.35771700	-1.02798700
S	5.46921600	-0.11960900	-0.53012700
C	3.10239400	-2.47937700	0.89747500
C	1.80271400	-3.26193700	0.95753600
H	0.74159200	-1.75415400	2.08322600
C	-0.65314700	-3.29763900	1.52813700
C	6.26415300	2.28305100	-1.11019700
C	4.09867400	3.63943800	-1.26130300
C	6.74863900	0.99509200	-0.86605000
H	3.20430700	-1.85432000	1.80176300
C	4.30488400	-3.38519200	0.74779800
H	1.66409400	-3.82333500	0.01939900
H	1.90407900	-4.00183600	1.76692700
H	-0.48418800	-3.87754100	2.44555400
H	-1.54382400	-2.67233700	1.67012800
H	-0.84058800	-4.00176400	0.70520400
C	7.15500900	3.47383000	-1.35286800
H	4.63716400	4.22753700	-2.01800800
H	3.12362900	3.42578800	-1.72177500
C	3.91452700	4.48682200	-0.00043200
H	4.22523000	-3.97823000	-0.17482500
H	5.23470200	-2.80451700	0.71360700
H	4.35741300	-4.07621000	1.59995600
H	7.84397100	3.26737600	-2.18513700
H	6.54472800	4.32238600	-1.68830600
C	7.95602400	3.88829600	-0.11739700
H	3.37122100	3.93604900	0.78126700
H	4.88547700	4.78831100	0.41811600
H	3.34658200	5.39968100	-0.23074700
H	8.57768700	4.76745400	-0.34037200
H	7.29006900	4.14526300	0.71945800
H	8.62092900	3.07976400	0.21891000
C	8.10646200	0.49186900	-0.90600800
S	9.27135800	1.04107700	-2.08802600
C	8.65760100	-0.52415500	-0.13817500
C	10.47860100	-0.03505500	-1.50491900
C	10.01725000	-0.81708300	-0.48034000
O	7.95062500	-1.19548100	0.79823700
O	10.75299700	-1.81127800	0.07132600
C	8.50737000	-1.20541400	2.13707200

C	10.94086600	-1.75647600	1.50083200
C	9.68027100	-2.16722600	2.24657700
H	8.84688400	-0.17818900	2.35975200
C	7.36795200	-1.57695600	3.06084000
H	11.20523100	-0.71664100	1.76644400
C	12.11022900	-2.67138900	1.79472000
H	9.36281000	-3.16581000	1.90379700
H	9.93734100	-2.25597600	3.31413100
H	7.70281400	-1.53616300	4.10624300
H	6.52798500	-0.88117300	2.93675000
H	7.01468600	-2.59707900	2.85110000
H	11.86727900	-3.70804400	1.51841500
H	12.99480200	-2.35707600	1.22509600
H	12.35632500	-2.64603000	2.86490400
C	-8.79383500	0.00263500	-0.13049100
C	-9.56870600	0.97778400	0.51122500
S	-9.81991800	-1.22201900	-0.85783200
C	-10.97271900	0.72833700	0.38794100
C	-9.03102100	2.14905800	1.28692600
C	-11.23155000	-0.41766400	-0.32562300
C	-12.07330400	1.58648000	0.95163300
H	-8.25171700	2.66844800	0.70776400
H	-9.83633500	2.88796700	1.40129000
C	-8.49223700	1.78018800	2.67205300
H	-12.20824900	-0.83186600	-0.56948500
H	-11.82720700	2.65035000	0.80689200
H	-12.98303800	1.40600300	0.35974100
C	-12.37689100	1.32448900	2.42631200
H	-8.13118100	2.67810100	3.19424300
H	-9.27539700	1.31876000	3.29023600
H	-7.65700300	1.06831100	2.60759500
H	-12.65010400	0.27137100	2.58998300
H	-11.51261800	1.54947300	3.06767500
H	-13.21573000	1.95025100	2.76470200
H	11.46220600	-0.06919600	-1.96525900

D. DSDSDA

a. Neutral

C	-1.01611600	0.86920600	0.20798100
C	-1.59167600	1.96202300	0.83342100
C	-3.02099300	1.97504400	0.71880500
C	-3.52270700	0.87835900	0.01951800
S	-2.21701600	-0.14877500	-0.52485700
C	-4.88878000	0.50061000	-0.29453400
C	-5.31030400	-0.53049600	-1.11967200
S	-6.29168300	1.33731700	0.33390300
C	-6.72965700	-0.63669100	-1.24240100

C	-7.41725800	0.28154000	-0.47605300
C	-0.80134400	2.98857400	1.60516100
H	0.00659400	3.39254200	0.97706200
H	-1.44588300	3.84656400	1.83933100
C	-3.85842900	3.08024500	1.30409400
H	-3.30408000	4.02671400	1.21513000
H	-4.76149700	3.22692800	0.69395200
C	-4.24890900	2.86231200	2.76674200
H	-4.82338100	1.93272000	2.89310700
H	-3.35915400	2.79330700	3.40974000
H	-4.86672100	3.69547600	3.13338800
C	-0.20091400	2.43950700	2.89992900
H	0.34598000	3.22737400	3.43888000
H	-0.98325900	2.05019600	3.56850900
H	0.50226400	1.61906900	2.69432700
O	-4.43195800	-1.30902400	-1.79793400
O	-7.36071100	-1.48410600	-2.09125400
C	-4.55133000	-2.74565100	-1.64739400
C	-7.12496800	-2.89706500	-1.91125000
C	-5.74652000	-3.28613200	-2.42380700
H	-7.21772800	-3.12141100	-0.83478900
H	-5.66289400	-2.96100600	-3.47296000
H	-5.67324700	-4.38563600	-2.42098200
C	-8.23448300	-3.59770900	-2.66644000
H	-8.15365200	-4.68587000	-2.53967200
H	-9.21547100	-3.27401100	-2.29451100
H	-8.17443900	-3.36750000	-3.74046300
C	-4.49339300	-3.16374700	-0.18917300
H	-5.34212400	-2.77475000	0.39120000
H	-4.50800900	-4.26070000	-0.11790800
H	-3.56700600	-2.79905900	0.27419600
H	-3.64356800	-3.10313200	-2.15283600
C	0.38775900	0.52500600	0.04655400
S	1.55641800	1.69985700	-0.49326600
C	0.98969600	-0.71085500	0.16404200
C	2.87410600	0.54926100	-0.49774100
C	2.38801900	-0.69553500	-0.12459800
O	0.29096400	-1.83263800	0.46145400
C	4.23777700	0.90273500	-0.84755700
O	3.16959500	-1.80448100	-0.10992600
C	0.71217300	-2.55404000	1.63939100
C	4.77439200	2.08950800	-1.34394900
S	5.49526800	-0.28669400	-0.61919800
C	3.23736500	-2.54443000	1.13285500
C	1.97383900	-3.35740400	1.36967800
H	0.90669900	-1.81334900	2.43601800

C	-0.45769600	-3.43095400	2.03120300
C	6.19888500	2.03655500	-1.50621500
C	3.97665900	3.31824400	-1.68908000
C	6.73056800	0.80844100	-1.15261400
H	3.36738000	-1.81265300	1.95029300
C	4.46397100	-3.42628100	1.02888900
H	1.80222600	-4.02063200	0.50579000
H	2.15495700	-4.00236800	2.24429500
H	-0.22446200	-3.99052300	2.94732000
H	-1.35237700	-2.82127200	2.21313100
H	-0.68219500	-4.15253700	1.23183300
C	7.03597400	3.20899200	-1.95216600
H	4.42903700	3.79546500	-2.57163100
H	2.96731800	3.02799800	-2.01510100
C	3.88232500	4.34236400	-0.55686100
H	4.36595100	-4.12009400	0.18091400
H	5.37006800	-2.82446600	0.88616400
H	4.57996200	-4.01777900	1.94737100
H	7.67659700	2.91584800	-2.79739900
H	6.38003200	3.99816100	-2.34366100
C	7.90930200	3.78630700	-0.83755000
H	3.41292100	3.90753200	0.33798400
H	4.87861200	4.70645800	-0.26591800
H	3.28238700	5.21100900	-0.86641100
H	8.48515300	4.64944100	-1.20319500
H	7.29826200	4.12128300	0.01401000
H	8.62265500	3.03723900	-0.46342200
C	8.10393000	0.32896000	-1.21802100
S	9.10928200	0.59127400	-2.62300500
C	8.77738100	-0.45448600	-0.30070100
C	10.43089700	-0.27537200	-1.93592100
C	10.11033100	-0.79203400	-0.71082100
O	8.20082400	-0.90712900	0.84031200
O	10.94712800	-1.59625300	-0.00758200
C	8.87094000	-0.56299100	2.07254500
C	11.26507800	-1.16917000	1.33227900
C	10.11040200	-1.41804700	2.29205800
H	9.16097200	0.50155400	2.01006200
C	7.84371700	-0.74842500	3.16919300
H	11.48959500	-0.08721500	1.29774700
C	12.51136900	-1.93610100	1.72083000
H	9.82615200	-2.48253800	2.24766300
H	10.47531200	-1.22056500	3.31280400
H	8.26498200	-0.45302400	4.13980200
H	6.95521400	-0.13423200	2.97242900
H	7.53369600	-1.80204700	3.23266000

H	12.30640000	-3.01669000	1.74414200
H	13.31633000	-1.75033400	0.99728600
H	12.85808500	-1.62722600	2.71633700
C	-8.85492000	0.48903700	-0.38507700
C	-9.63895700	0.78045300	0.72096000
S	-9.81553100	0.43520800	-1.84005200
C	-11.02342000	0.96329000	0.37581400
C	-9.12083100	0.84793900	2.13541900
C	-11.24796000	0.80708000	-0.96879400
C	-12.12846100	1.26453900	1.35223200
H	-8.28451600	1.56049800	2.20036400
H	-9.90719000	1.26218500	2.78231000
C	-8.66993900	-0.50558400	2.68534800
H	-12.19861300	0.88052400	-1.49336900
H	-11.79856200	2.04524400	2.05677600
H	-12.97407100	1.69781200	0.79703500
C	-12.61335700	0.04297500	2.13254300
H	-8.32018800	-0.40677400	3.72369700
H	-9.49287700	-1.23585500	2.67147600
H	-7.84488300	-0.92039900	2.08783700
H	-12.98450000	-0.73607000	1.44979300
H	-11.80780700	-0.40002500	2.73658900
H	-13.43204000	0.31594600	2.81500300
H	11.36887800	-0.38473400	-2.47306000

b. Radical Cation

C	0.97837100	-0.94041000	0.10357300
C	1.64421600	-2.15597900	0.41199000
C	3.04420800	-2.03798600	0.39295100
C	3.48756000	-0.72830000	0.07466600
S	2.13138000	0.34998300	-0.16574200
C	4.81116400	-0.23313200	-0.10475200
C	5.19001300	1.09480000	-0.36695600
S	6.24183800	-1.24648900	-0.11429100
C	6.57715800	1.26804600	-0.56735400
C	7.31338500	0.08886400	-0.43350000
C	0.93374900	-3.42689600	0.78529900
H	0.11925900	-3.62643100	0.07396400
H	1.61980700	-4.27369000	0.66137600
C	3.96727900	-3.17874300	0.71953600
H	3.45097700	-4.12753100	0.52576400
H	4.81671000	-3.18433400	0.02187500
C	4.46972500	-3.16675600	2.16512000
H	5.01164900	-2.23917700	2.39935100
H	3.63365000	-3.25451200	2.87337400
H	5.15223100	-4.01092900	2.33876900
C	0.39645700	-3.42637700	2.21893800

H	-0.12218100	-4.37215900	2.43083100
H	1.21430800	-3.31651800	2.94506600
H	-0.31450900	-2.60496800	2.38756200
O	4.26938700	2.06726300	-0.47531900
O	7.16371800	2.42097500	-0.95350300
C	4.45232900	3.28833400	0.29821300
C	6.98973400	3.58806100	-0.11177000
C	5.58267200	4.14114700	-0.25814800
H	7.18727500	3.28149100	0.92862900
H	5.39240900	4.33396400	-1.32544900
H	5.53895100	5.11421100	0.25618800
C	8.04261600	4.57939300	-0.55642700
H	7.98885000	5.48575500	0.06162500
H	9.04648900	4.14763100	-0.45630000
H	7.88472900	4.86477300	-1.60670800
C	4.53857600	2.97850700	1.78066000
H	5.42950900	2.38703500	2.03505400
H	4.58059000	3.91666500	2.35161700
H	3.65251900	2.41636800	2.10557400
H	3.51288200	3.81800000	0.09626400
C	-0.40849800	-0.68336500	-0.05522600
S	-1.61732500	-1.94666900	-0.15474500
C	-1.03230300	0.56915200	-0.24360600
C	-2.92276900	-0.82257300	-0.42781800
C	-2.42011400	0.49222800	-0.45114800
O	-0.30483300	1.69700100	-0.27731800
C	-4.27960000	-1.23178000	-0.60789400
O	-3.22454100	1.52542400	-0.76763900
C	-0.73331000	2.80631300	0.55995000
C	-4.83385400	-2.51812700	-0.75508200
S	-5.53829800	-0.01757100	-0.61874900
C	-3.24833000	2.69874900	0.08542800
C	-1.95738100	3.48933200	-0.01869500
H	-0.96964600	2.38959100	1.55428800
C	0.45916700	3.72926400	0.65804000
C	-6.25018100	-2.50403200	-0.85056400
C	-4.03662700	-3.79085500	-0.82351300
C	-6.78170100	-1.21122800	-0.78986900
H	-3.38855900	2.34925400	1.12337100
C	-4.44756100	3.50478300	-0.36339900
H	-1.76749300	3.75439100	-1.07137500
H	-2.10437000	4.43090500	0.53297200
H	0.22198000	4.57774400	1.31352100
H	1.32025800	3.19541800	1.07832900
H	0.72965600	4.11962100	-0.33369600
C	-7.08915200	-3.75244200	-0.93460200

H	-4.53051900	-4.47446000	-1.52924300
H	-3.05365900	-3.58989000	-1.27286800
C	-3.86452000	-4.49569600	0.52397800
H	-4.32498600	3.82423700	-1.40843400
H	-5.37110600	2.91905700	-0.28032000
H	-4.54704200	4.40120100	0.26340900
H	-7.79034300	-3.68337600	-1.77936200
H	-6.44157700	-4.60662800	-1.17159500
C	-7.86262100	-4.05074400	0.35109400
H	-3.36867800	-3.84642300	1.26037100
H	-4.83577800	-4.79329200	0.94415700
H	-3.25482000	-5.40301200	0.40590600
H	-8.44057300	-4.98000100	0.24366100
H	-7.18048100	-4.17050900	1.20547700
H	-8.56602500	-3.24151900	0.59420600
C	-8.15412800	-0.76379700	-0.89770500
S	-9.34386800	-1.59210700	-1.87611000
C	-8.71217200	0.38842600	-0.35901800
C	-10.56188000	-0.43728000	-1.50518200
C	-10.09014900	0.56648100	-0.70261400
O	-7.99406400	1.27391100	0.36680100
O	-10.83601600	1.64307500	-0.35862200
C	-8.49725300	1.57833900	1.69244100
C	-10.97083400	1.90946300	1.05324600
C	-9.69862500	2.50865700	1.63310500
H	-8.78900500	0.62158700	2.16076100
C	-7.33584600	2.18433900	2.44995200
H	-11.19247900	0.95136200	1.55755900
C	-12.15752700	2.84025700	1.18103900
H	-9.42927600	3.41228500	1.06185200
H	-9.91978900	2.82910600	2.66364200
H	-7.62495600	2.37505800	3.49239300
H	-6.47517000	1.50293800	2.44558600
H	-7.03236400	3.13867600	1.99552700
H	-11.95700500	3.79238800	0.66805300
H	-13.05095900	2.38476700	0.73380200
H	-12.36554600	3.05252300	2.23847700
C	8.73260000	-0.08314100	-0.61382400
C	9.56412300	-1.15369000	-0.26595300
S	9.64202300	1.16599000	-1.44304400
C	10.91634500	-0.95348000	-0.69124500
C	9.13967200	-2.37013400	0.51234600
C	11.08076800	0.24747100	-1.33972300
C	12.05670500	-1.91083900	-0.47215300
H	8.23909800	-2.81932200	0.06595800
H	9.91895300	-3.13783400	0.40793400

C	8.90216700	-2.09662500	1.99956100
H	12.00130900	0.64283300	-1.76540900
H	11.71805300	-2.94180400	-0.66206500
H	12.82796200	-1.70376700	-1.22897600
C	12.68362700	-1.82282900	0.91883300
H	8.61628000	-3.02249400	2.51950600
H	9.81030400	-1.70339700	2.47866700
H	8.09925500	-1.36133000	2.15264000
H	13.05442800	-0.80643000	1.11857000
H	11.96203100	-2.07671400	1.70885100
H	13.53182200	-2.51773100	1.00519400
H	-11.56115500	-0.53105100	-1.92134900

E. DSDADS

a. Neutral

C	-1.05743000	1.05451800	-0.30962000
C	-1.65952800	2.30905400	-0.30737600
C	-3.08810600	2.24474700	-0.41246100
C	-3.56485700	0.94224000	-0.48113500
S	-2.25914300	-0.20532100	-0.41644500
C	-4.92301700	0.43561700	-0.55927600
C	-5.37398400	-0.71448100	-1.18252200
S	-6.26226200	1.23805800	0.22274700
C	-6.77539200	-0.93558100	-1.02835300
C	-7.41742700	0.02412500	-0.26578300
C	-0.91574400	3.61275700	-0.17327200
H	-0.09112000	3.66071300	-0.90096700
H	-1.58608800	4.43663100	-0.45408800
C	-3.96329300	3.46722600	-0.49145500
H	-3.48743800	4.20196100	-1.16038000
H	-4.91080600	3.19642700	-0.97964100
C	-4.25942500	4.13030500	0.85442900
H	-4.74724800	3.42884600	1.54755600
H	-3.34141000	4.48978100	1.34096500
H	-4.92815600	4.99347200	0.72047200
C	-0.37395800	3.86517600	1.23528000
H	0.14441800	4.83426300	1.28403400
H	-1.18743800	3.87655600	1.97554200
H	0.33988300	3.08497500	1.53652900
O	-4.56651600	-1.49871800	-1.93725400
O	-7.44789100	-1.93686600	-1.64721800
C	-4.50336600	-2.90099500	-1.59235300
C	-7.03616900	-3.28429700	-1.32477400
C	-5.74811900	-3.64892600	-2.04534400
H	-4.40774500	-2.97312600	-0.49372200
H	-6.88022700	-3.33457600	-0.23212500
H	-5.88676700	-3.49872900	-3.12881400

H	-5.56663300	-4.72385700	-1.88601200
C	-3.24865500	-3.43066400	-2.25385200
H	-3.32019400	-3.32910100	-3.34689200
H	-2.36507700	-2.87872300	-1.90864300
H	-3.11266600	-4.49388600	-2.01314200
C	-8.19088400	-4.17973000	-1.72010600
H	-7.96144100	-5.22570600	-1.47501800
H	-9.10544300	-3.88764200	-1.18794300
H	-8.37810700	-4.11031700	-2.80186400
C	0.34388400	0.67904600	-0.30461400
S	1.61931200	1.76529200	-0.80288700
C	0.88707400	-0.56521500	-0.03506200
C	2.87789700	0.56734200	-0.59927400
C	2.30268400	-0.62346300	-0.18553100
O	0.11649100	-1.64268500	0.25500400
C	4.28274100	0.82783000	-0.85124400
O	3.03257800	-1.75373100	-0.02189600
C	0.37753300	-2.31470900	1.50948100
C	4.93112900	1.97970300	-1.29598300
S	5.43805000	-0.45735900	-0.58063100
C	2.95341800	-2.42994100	1.25748900
C	1.63039000	-3.17108500	1.40792700
H	0.49613300	-1.54032900	2.28621600
C	-0.85488400	-3.14208200	1.80668900
C	6.35469800	1.82308600	-1.38261700
C	4.24571500	3.27017000	-1.65635000
C	6.77325300	0.55473500	-1.02639100
C	3.30287500	-1.50071800	2.40567600
H	3.74423000	-3.18701100	1.16385600
H	1.51020300	-3.85839300	0.55560600
H	1.69905600	-3.79249900	2.31524200
H	-0.74077300	-3.65553700	2.77116800
H	-1.74651600	-2.50362100	1.85337100
H	-1.00726000	-3.90191800	1.02589600
C	7.31126900	2.92762400	-1.75356600
H	4.80768900	3.75155200	-2.47057400
H	3.25642600	3.06052800	-2.08843100
C	4.10694300	4.25377100	-0.49326400
H	2.58168500	-0.67772900	2.51290400
H	3.31494600	-2.06592600	3.34855600
H	4.29911700	-1.06487100	2.25103800
H	8.02346900	2.56391200	-2.50896900
H	6.76137500	3.74861600	-2.23368200
C	8.09256400	3.47009600	-0.55621000
H	3.52970800	3.81596500	0.33445000
H	5.09168500	4.54218200	-0.09741100

H	3.59225400	5.17024300	-0.81807000
H	8.76717500	4.28170400	-0.86705400
H	7.41760500	3.86652900	0.21690900
H	8.70242000	2.67965500	-0.09428700
C	8.11534300	-0.01463700	-1.03014800
S	9.10320900	-0.01497000	-2.47070600
C	8.75783700	-0.69678600	-0.01742500
C	10.38424600	-0.85670600	-1.68330700
C	10.05887200	-1.17451700	-0.39318800
O	8.17900400	-0.93573000	1.18495700
O	10.85861800	-1.92739200	0.40396600
C	8.90441100	-0.47291800	2.34439400
C	11.23334600	-1.34284400	1.66703600
C	10.08578600	-1.37657700	2.66619300
H	9.26940700	0.54754500	2.12734600
C	7.89280400	-0.42356000	3.46975400
H	11.52827000	-0.29389900	1.47996400
C	12.43465500	-2.13259000	2.14199900
H	9.72904400	-2.41441900	2.77328200
H	10.48577700	-1.06690800	3.64501800
H	8.35894100	-0.03683000	4.38623200
H	7.05223100	0.23045800	3.20264500
H	7.49982200	-1.42972600	3.67834900
H	12.16022200	-3.18393800	2.31430700
H	13.23490300	-2.10084300	1.39060600
H	12.82118200	-1.71650000	3.08234400
C	-8.83781600	0.13253000	0.02438700
C	-9.49796300	0.80217700	1.04849000
S	-9.98183200	-0.61572800	-1.06731400
C	-10.92853800	0.71411800	0.92913300
C	-8.82196300	1.51307400	2.19265900
C	-11.31363100	-0.01450300	-0.16670800
C	-11.92149900	1.32481000	1.88146600
H	-8.07158300	2.22421600	1.81403400
H	-9.56720100	2.13495400	2.70885500
C	-8.16751100	0.56987600	3.20373400
H	-12.32900500	-0.24316700	-0.48482800
H	-11.60710400	2.34893200	2.14039400
H	-12.88307900	1.42966000	1.35660700
C	-12.13545400	0.51669300	3.16092400
H	-7.71010000	1.13944100	4.02630800
H	-8.90596600	-0.12039800	3.63778200
H	-7.37954600	-0.03629600	2.73397300
H	-12.48455600	-0.50054500	2.92818300
H	-11.20793900	0.42500100	3.74490400
H	-12.88893800	0.99649600	3.80322100

H	11.30212000	-1.10234500	-2.21023800
b. Radical Cation			
C	-1.01618900	1.11789000	-0.10913600
C	-1.70702500	2.35332000	-0.09978000
C	-3.10157300	2.20593600	-0.23073700
C	-3.50497200	0.85466300	-0.34534000
S	-2.13075800	-0.21634600	-0.28488400
C	-4.81189300	0.29376400	-0.47269800
C	-5.14327800	-1.00025200	-0.90063900
S	-6.27363900	1.17075800	-0.08223600
C	-6.53378500	-1.25766700	-0.89691100
C	-7.30565700	-0.18350300	-0.44569900
C	-1.04268300	3.68726600	0.10050200
H	-0.19484100	3.79886300	-0.59182900
H	-1.74480200	4.48100600	-0.18495200
C	-4.04429900	3.37700000	-0.28864100
H	-3.56058100	4.18897600	-0.85135800
H	-4.92477700	3.10526800	-0.88782200
C	-4.48708000	3.90370800	1.07793300
H	-4.97235000	3.11995900	1.67775700
H	-3.63324200	4.28344900	1.65639300
H	-5.20365300	4.72830400	0.95416100
C	-0.57891900	3.92499500	1.54048600
H	-0.11232300	4.91630000	1.63025700
H	-1.42612200	3.88178900	2.23964000
H	0.15731000	3.17432100	1.86086300
O	-4.19305600	-1.82813000	-1.36943400
O	-7.11637800	-2.37830300	-1.37076400
C	-4.14164500	-3.20696200	-0.91672100
C	-6.67162200	-3.64868900	-0.83700800
C	-5.31947600	-4.02531500	-1.41419600
H	-4.14158700	-3.18858000	0.18730700
H	-6.59803600	-3.54292200	0.25969600
H	-5.36800300	-3.97488700	-2.51413600
H	-5.11871700	-5.07419700	-1.14528000
C	-2.82474400	-3.74372000	-1.43466800
H	-2.82036600	-3.74851000	-2.53431000
H	-1.98376400	-3.13326600	-1.08404900
H	-2.67740700	-4.77376400	-1.08324400
C	-7.74951300	-4.65014500	-1.18955900
H	-7.48567100	-5.63927700	-0.79165800
H	-8.71463300	-4.34913900	-0.76305100
H	-7.85718000	-4.73221300	-2.28089900
C	0.37833900	0.85172200	-0.05873400
S	1.59885600	2.05175200	-0.42092700
C	0.99963600	-0.38514600	0.20093000

C	2.92025300	0.92756500	-0.19696500
C	2.40104300	-0.33729700	0.14266700
O	0.27539600	-1.49527000	0.43572700
C	4.29083000	1.26395200	-0.39959300
O	3.21482300	-1.39594300	0.31122500
C	0.53443200	-2.21396900	1.67509100
C	4.88545100	2.50751900	-0.70155700
S	5.50773200	0.00381100	-0.31336400
C	3.11587200	-2.14662600	1.55328700
C	1.84334500	-2.98014300	1.58881100
H	0.56902700	-1.46466300	2.48239900
C	-0.65121700	-3.12800500	1.88740800
C	6.29043200	2.42861000	-0.85279300
C	4.12757800	3.79896100	-0.83174700
C	6.78268600	1.12089800	-0.70020100
C	3.33459200	-1.24798700	2.75582700
H	3.96357700	-2.83791200	1.46284200
H	1.81243600	-3.62657200	0.69801000
H	1.90846400	-3.64393800	2.46538600
H	-0.55299800	-3.64114900	2.85363500
H	-1.58666700	-2.55409000	1.89156000
H	-0.70423800	-3.88927000	1.09621400
C	7.16350000	3.63398300	-1.08108300
H	4.67522700	4.46710500	-1.50971800
H	3.17030000	3.62126300	-1.34206400
C	3.89279100	4.51348200	0.50095500
H	2.54052900	-0.49676200	2.87169500
H	3.36059300	-1.85658700	3.67062200
H	4.29204000	-0.71736800	2.66748100
H	7.84705300	3.45601000	-1.92397200
H	6.53942100	4.47735900	-1.40229900
C	7.95855200	4.04961600	0.15871400
H	3.33140700	3.88218700	1.20503300
H	4.84638200	4.78066600	0.97827100
H	3.32076800	5.43909600	0.34368300
H	8.57231600	4.93542800	-0.05952100
H	7.28631000	4.29847000	0.99264100
H	8.63050600	3.24792900	0.49683200
C	8.12418700	0.61561000	-0.86938700
S	9.35221200	1.46700700	-1.78550000
C	8.62786800	-0.61761600	-0.45757800
C	10.49770400	0.20886600	-1.56583400
C	9.98197700	-0.84347500	-0.85738300
O	7.86601600	-1.52349200	0.18961100
O	10.67076000	-1.99152400	-0.66175100
C	8.38008500	-2.04734800	1.44240800

C	10.81139800	-2.44116100	0.70154800
C	9.51330400	-3.03632100	1.22153100
H	8.74527200	-1.18743800	2.03092200
C	7.19568300	-2.68154300	2.13719800
H	11.09243100	-1.56801700	1.31810500
C	11.94549700	-3.44296200	0.68733200
H	9.17620700	-3.83117200	0.53621600
H	9.72609700	-3.51141800	2.19221700
H	7.49735200	-3.06766300	3.12008300
H	6.39647100	-1.94470800	2.28362100
H	6.80235400	-3.51780300	1.54098000
H	11.68583300	-4.31109500	0.06376000
H	12.85677700	-2.98312000	0.28263500
H	12.15549200	-3.79714000	1.70560200
C	-8.74352600	-0.11625900	-0.35233700
C	-9.56768000	0.85567400	0.22610600
S	-9.70677500	-1.37843200	-1.09945200
C	-10.95984200	0.57383400	0.03960800
C	-9.09154200	2.05604100	0.99844500
C	-11.16055900	-0.59294800	-0.65723700
C	-12.10317400	1.42246400	0.52755200
H	-8.29839400	2.58025700	0.44282200
H	-9.91690200	2.77902500	1.05995500
C	-8.60662200	1.73006800	2.41381900
H	-12.11517700	-1.03428000	-0.93795700
H	-11.87311300	2.48722500	0.36351400
H	-12.98082800	1.20534700	-0.09949300
C	-12.46827300	1.19554700	1.99403000
H	-8.28603400	2.64654800	2.93030100
H	-9.40651000	1.26656700	3.00876800
H	-7.75560400	1.03413300	2.40167300
H	-12.72874100	0.14207400	2.17541500
H	-11.63769300	1.45513400	2.66601900
H	-13.33297100	1.81352700	2.27733500
H	11.49193400	0.28243700	-1.99794100

F. DSDADA

a. Neutral

C	-1.01680900	0.82418800	0.13509700
C	-1.57576200	1.96520200	0.68114600
C	-3.00436100	1.99524500	0.55484900
C	-3.51968300	0.86215300	-0.07241700
S	-2.22791500	-0.21852000	-0.54109200
C	-4.89054900	0.48300200	-0.36406700
C	-5.32447800	-0.58552700	-1.13296000
S	-6.28209700	1.36080800	0.23153300
C	-6.74570700	-0.68644600	-1.24118300

C	-7.42055400	0.27422300	-0.51686500
C	-0.76681700	3.02327400	1.38776500
H	0.06138300	3.35386800	0.74313500
H	-1.38878300	3.91407600	1.55047200
C	-3.82496100	3.15459100	1.05251700
H	-3.25622600	4.08254100	0.88833100
H	-4.72721700	3.26494300	0.43350400
C	-4.21612200	3.06066400	2.52815500
H	-4.80015800	2.15065800	2.73025800
H	-3.32699500	3.03570300	3.17520200
H	-4.82497800	3.92748300	2.82519500
C	-0.19768800	2.55091400	2.72624700
H	0.36947400	3.35767400	3.21387600
H	-0.99813600	2.23522000	3.41202800
H	0.47987000	1.69549600	2.58730900
O	-4.45473400	-1.40297900	-1.77560200
O	-7.39016500	-1.57005500	-2.04160600
C	-4.58475800	-2.83023500	-1.55906000
C	-7.16146200	-2.97386700	-1.79443700
C	-5.79043300	-3.39619700	-2.30031400
H	-7.24528900	-3.14428000	-0.70739600
H	-5.71394700	-3.11995600	-3.36390400
H	-5.72457800	-4.49491900	-2.24765400
C	-8.28257800	-3.70311600	-2.50399400
H	-8.20778600	-4.78425500	-2.32453500
H	-9.25783600	-3.35447300	-2.13956300
H	-8.23105300	-3.52638600	-3.58854500
C	-4.51785300	-3.18429900	-0.08409400
H	-5.35141300	-2.75248900	0.48815300
H	-4.55500400	-4.27654500	0.03527500
H	-3.57843900	-2.82110300	0.35361800
H	-3.68422700	-3.21766400	-2.05527100
C	0.38397000	0.44552800	0.01989800
S	1.55119400	1.50490300	-0.72400300
C	0.97794000	-0.75511800	0.34480000
C	2.86425900	0.36340200	-0.53599600
C	2.37649000	-0.79234700	0.05439300
O	0.27044800	-1.80682100	0.82382700
C	4.22873500	0.62959400	-0.95678800
O	3.16111000	-1.87863700	0.26169000
C	0.67977300	-2.34220400	2.10084900
C	4.77567200	1.71600400	-1.63743200
S	5.46845800	-0.54788300	-0.58995600
C	3.22412000	-2.41431500	1.60701200
C	1.94877800	-3.17021700	1.96199600
H	0.84157300	-1.49314400	2.78676800

C	-0.48937400	-3.16864200	2.59319700
C	6.19399000	1.60333600	-1.82598100
C	3.99579900	2.90093000	-2.14017000
C	6.70771800	0.42953100	-1.30799100
C	3.64368300	-1.35781200	2.61335400
H	4.03028100	-3.15571500	1.51845700
H	1.77328200	-3.94581000	1.19963400
H	2.12827100	-3.69178800	2.91592000
H	-0.27434400	-3.57868800	3.58938500
H	-1.39539300	-2.55166900	2.65734200
H	-0.68398800	-4.00629600	1.90718500
C	7.05337900	2.66744600	-2.46036000
H	4.44085700	3.23804300	-3.08861900
H	2.97474500	2.59123900	-2.40629100
C	3.94406500	4.07742700	-1.16435400
H	2.90688700	-0.54642000	2.70106900
H	3.76085500	-1.81784400	3.60497700
H	4.60559800	-0.91539300	2.32143800
H	7.69794600	2.21571100	-3.22900400
H	6.41669500	3.38740300	-2.99250300
C	7.92995800	3.41163400	-1.45225600
H	3.48841900	3.78392600	-0.20712400
H	4.95252800	4.46037200	-0.94965000
H	3.35119500	4.90428400	-1.58278200
H	8.52620400	4.18824900	-1.95400100
H	7.32191500	3.89890500	-0.67544600
H	8.62413900	2.72167100	-0.95016100
C	8.07529200	-0.07503100	-1.33053000
S	8.96134200	-0.26155100	-2.82390700
C	8.82474400	-0.55127800	-0.27443100
C	10.34165000	-0.89959900	-2.01271900
C	10.12436800	-1.01854600	-0.66733200
O	8.34207500	-0.61882500	0.99060000
O	11.02186200	-1.58823100	0.17652000
C	9.11171400	0.06166400	2.00497300
C	11.44052200	-0.78625300	1.29867100
C	10.36591700	-0.71652300	2.37410000
H	9.39571800	1.05153200	1.60357100
C	8.17538700	0.23791200	3.18168000
H	11.65508900	0.23207500	0.92545900
C	12.71840500	-1.42350400	1.80226400
H	10.08206600	-1.74027400	2.66932700
H	10.81025500	-0.23343100	3.25912000
H	8.67433900	0.79249600	3.98808700
H	7.27791000	0.79343400	2.87909900
H	7.86368900	-0.74102100	3.57514100

H	12.52305100	-2.44419500	2.16328100
H	13.46325100	-1.47583500	0.99698700
H	13.13936600	-0.83732600	2.63040500
C	-8.85619900	0.49623200	-0.42494700
C	-9.63065900	0.82760200	0.67630800
S	-9.82611800	0.40440800	-1.87146500
C	-11.01604300	1.00972400	0.33437300
C	-9.10099800	0.93543000	2.08393200
C	-11.25033400	0.81365500	-1.00337900
C	-12.11275600	1.34797300	1.30807300
H	-8.25796500	1.64211900	2.11930500
H	-9.87833500	1.37688400	2.72371500
C	-8.65675400	-0.40396400	2.67256200
H	-12.20386100	0.87764000	-1.52396000
H	-12.95911000	1.77001800	0.74541900
H	-11.77308600	2.14720200	1.98674900
C	-12.60029400	0.15362600	2.12778500
H	-8.29768000	-0.27567400	3.70448100
H	-9.48559400	-1.12750500	2.68809600
H	-7.84007600	-0.84413000	2.08163600
H	-11.79336000	-0.27680200	2.73899000
H	-12.98166300	-0.64274700	1.47115000
H	-13.41210600	0.45242800	2.80764100
H	11.23510700	-1.18212400	-2.56261500

b. Radical Cation

C	0.98122200	-1.00121600	0.30842200
C	1.68156700	-2.22717600	0.44620300
C	3.07466500	-2.08305600	0.32254300
C	3.47721500	-0.74184200	0.09985800
S	2.09572300	0.32993200	0.07518000
C	4.77804400	-0.20661000	-0.13464300
C	5.11903800	1.14478100	-0.30491600
S	6.21633900	-1.18723900	-0.34358200
C	6.48482000	1.36195500	-0.59428600
C	7.24386100	0.19084300	-0.62604900
C	1.01796400	-3.53895100	0.75981500
H	0.15887300	-3.69810800	0.09202500
H	1.70721000	-4.35819400	0.52163200
C	4.03237100	-3.23531300	0.44819000
H	3.51167400	-4.16662100	0.19070000
H	4.82186400	-3.14731200	-0.31165100
C	4.65085500	-3.37240700	1.84111600
H	5.19464900	-2.46275500	2.13409100
H	3.87735900	-3.55967400	2.59949900
H	5.35917000	-4.21287900	1.86379300
C	0.58299200	-3.66513100	2.22241900

H	0.10348200	-4.63940500	2.39368800
H	1.44744600	-3.58767000	2.89703700
H	-0.13388700	-2.88080700	2.50446100
O	4.18130500	2.10676400	-0.25702000
O	7.02315500	2.55670500	-0.92067900
C	4.40875300	3.25456500	0.60991100
C	6.90207700	3.64145400	0.03285800
C	5.48055700	4.17687700	0.04864500
H	7.18731500	3.24916000	1.02298400
H	5.20386700	4.46168800	-0.97843500
H	5.46535800	5.09809400	0.65239400
C	7.90121000	4.69030400	-0.40431300
H	7.88464700	5.53794200	0.29399300
H	8.91625400	4.27382400	-0.42352000
H	7.65415500	5.06287600	-1.40910100
C	4.61588500	2.81390000	2.04664900
H	5.53401700	2.22374200	2.17714700
H	4.68624700	3.69741000	2.69655100
H	3.76792300	2.20304900	2.38511600
H	3.44975500	3.78203000	0.53106000
C	-0.41629900	-0.75454600	0.27350700
S	-1.61208800	-2.02570500	0.10954700
C	-1.06675000	0.49712500	0.26101800
C	-2.95071100	-0.90514600	0.03355100
C	-2.46218700	0.41105900	0.13283600
O	-0.36436300	1.64310400	0.30098100
C	-4.30569000	-1.30320800	-0.17147300
O	-3.29524200	1.46243200	0.01685000
C	-0.71640600	2.62736400	1.31372400
C	-4.87618100	-2.59163300	-0.22501500
S	-5.52946600	-0.07681300	-0.44164100
C	-3.28151500	2.47375200	1.05984400
C	-2.02276000	3.32275600	0.97213800
H	-0.79634500	2.09091900	2.27293600
C	0.44647900	3.59142700	1.36807600
C	-6.26997700	-2.57163500	-0.47955000
C	-4.11241100	-3.86723900	-0.00360200
C	-6.77114800	-1.27250600	-0.65376100
C	-3.55967800	1.86340600	2.42044600
H	-4.13140900	3.10529100	0.77023100
H	-1.94359000	3.74399500	-0.04205600
H	-2.14594300	4.17060400	1.66410600
H	0.26559800	4.35132900	2.13998000
H	1.37301200	3.05916900	1.61515900
H	0.57336700	4.09983400	0.40137100
C	-7.12811300	-3.80936700	-0.48468300

H	-4.61438500	-4.68211100	-0.54219600
H	-3.12231300	-3.80009900	-0.47598300
C	-3.97065900	-4.24852200	1.47152300
H	-2.77023800	1.16876800	2.74040800
H	-3.63587800	2.65974200	3.17401700
H	-4.50929600	1.31242500	2.40325500
H	-7.73626200	-3.84951100	-1.40020100
H	-6.48395600	-4.69595500	-0.53722400
C	-8.03064500	-3.92419200	0.74556900
H	-3.45477700	-3.46348700	2.04344100
H	-4.95594400	-4.40674300	1.93312900
H	-3.39397500	-5.17895800	1.57402500
H	-8.62720900	-4.84667100	0.69831100
H	-7.43533400	-3.95097500	1.66992500
H	-8.72588900	-3.07557300	0.81789000
C	-8.09840500	-0.83824300	-1.02602100
S	-9.21480800	-1.86166400	-1.90605000
C	-8.65385500	0.42922800	-0.87393800
C	-10.39372000	-0.61787200	-2.00907800
C	-9.96400400	0.54909300	-1.43611100
O	-7.97472800	1.45054400	-0.30987600
O	-10.67972200	1.69616300	-1.49947800
C	-8.62360600	2.13856300	0.79067800
C	-10.96731500	2.35394100	-0.24869400
C	-9.73668600	3.05336200	0.30557200
H	-9.04171300	1.36592400	1.45983000
C	-7.52676600	2.89714300	1.50452200
H	-11.31069600	1.58467400	0.46678200
C	-12.09700900	3.31658200	-0.54497900
H	-9.33613200	3.74375900	-0.45480400
H	-10.05679300	3.66489900	1.16400400
H	-7.93645700	3.41694000	2.38099700
H	-6.74161200	2.20959200	1.84288000
H	-7.07768900	3.64560500	0.83533300
H	-11.77436400	4.07663900	-1.27168200
H	-12.95837100	2.77861800	-0.96252300
H	-12.41585200	3.82731100	0.37365900
C	8.64621100	0.06318600	-0.93561000
C	9.50893000	-1.02894600	-0.79177300
S	9.48079200	1.41972200	-1.67064200
C	10.82171500	-0.75752700	-1.29578200
C	9.15636800	-2.34066500	-0.14357000
C	10.92856900	0.51786200	-1.79624300
C	11.97782000	-1.72122000	-1.30140700
H	8.21762500	-2.73723800	-0.55998700
H	9.92116900	-3.08012100	-0.41886700

C	9.05862100	-2.26713800	1.38241500
H	11.80976000	0.97705100	-2.24066100
H	12.67783000	-1.41010500	-2.09112900
H	11.62390200	-2.72344900	-1.59118400
C	12.72828400	-1.80571400	0.02729500
H	8.82061700	-3.25614500	1.80027300
H	10.00814900	-1.93093400	1.82306400
H	8.27520000	-1.56674300	1.70544200
H	12.08121600	-2.16701200	0.83963100
H	13.11708900	-0.81970100	0.32249400
H	13.58002800	-2.49689900	-0.05372700
H	-11.33818200	-0.78952000	-2.51812100

G. DADADA

a. Neutral

C	1.00328800	-0.79134300	0.10970300
C	1.56037100	-1.97319100	0.56412000
C	2.98794000	-1.99895500	0.42718000
C	3.50501300	-0.82349600	-0.11559200
S	2.21531900	0.29573700	-0.49092600
C	4.87563600	-0.42933300	-0.38717300
C	5.31069400	0.70538500	-1.05396500
S	6.26604500	-1.37586800	0.09517000
C	6.73100500	0.80285400	-1.17292200
C	7.40665500	-0.23312100	-0.56109500
C	0.75168400	-3.08033800	1.19208300
H	-0.06634300	-3.37575700	0.51783700
H	1.37904500	-3.97499200	1.30373600
C	3.80703100	-3.19348600	0.83604300
H	3.23073400	-4.10570500	0.61935400
H	4.70015300	-3.26909000	0.19895800
C	4.21754200	-3.19706800	2.30939200
H	4.81199700	-2.30633400	2.56100700
H	3.33656000	-3.20609500	2.96802400
H	4.82252600	-4.08578300	2.54288600
C	0.16483900	-2.70131700	2.55215800
H	-0.40102300	-3.54266300	2.97902200
H	0.95576500	-2.42631700	3.26601200
H	-0.51807100	-1.84367600	2.46229700
O	4.44121500	1.58738900	-1.60495300
O	7.37257100	1.75659900	-1.89097200
C	4.58384900	2.98687300	-1.25604200
C	7.15940700	3.13057800	-1.50174500
C	5.78802800	3.61232000	-1.95043900
H	7.25350500	3.18945300	-0.40388700
H	5.69987600	3.44163400	-3.03506800
H	5.73302300	4.70116000	-1.79021800

C	8.28113500	3.91826800	-2.14461700
H	8.21752400	4.97646200	-1.85677800
H	9.25611100	3.52671200	-1.82596600
H	8.21905000	3.85196100	-3.24094300
C	4.53066700	3.20068600	0.24609800
H	5.36900100	2.71696600	0.76740000
H	4.56980500	4.27685400	0.46770300
H	3.59489800	2.79814100	0.65643300
H	3.68254500	3.42544300	-1.70617000
C	-0.39654500	-0.40116100	0.02803800
S	-1.57116400	-1.41187000	-0.76983500
C	-0.98570400	0.77927100	0.42785000
C	-2.88034200	-0.28097700	-0.50616900
C	-2.38584900	0.83702400	0.14799600
O	-0.27336800	1.79853800	0.96642500
C	-4.24720600	-0.51881900	-0.93607300
O	-3.16602400	1.91197500	0.42150800
C	-0.67768500	2.25737000	2.27448000
C	-4.80128200	-1.56865600	-1.66671700
S	-5.47953000	0.64797800	-0.51341000
C	-3.22217000	2.36987200	1.79545900
C	-1.94229200	3.09900800	2.18826400
H	-0.84399600	1.36910200	2.90765900
C	0.49698200	3.04464900	2.81519500
C	-6.21892000	-1.43825100	-1.84857200
C	-4.02990700	-2.73314100	-2.22707200
C	-6.72494900	-0.28605000	-1.27730400
C	-3.64240800	1.25877900	2.74067700
H	-4.02572200	3.11809400	1.75271000
H	-1.76531400	3.91578100	1.47064500
H	-2.11584700	3.56588500	3.17116600
H	0.28655300	3.39129300	3.83615000
H	1.39947500	2.41967200	2.83749300
H	0.69528300	3.92348900	2.18388200
C	-7.08581900	-2.46753800	-2.52883800
H	-4.48214900	-3.02431800	-3.18717500
H	-3.00897700	-2.41671900	-2.48521600
C	-3.97829100	-3.95312000	-1.30625300
H	-2.90778000	0.44180600	2.77941600
H	-3.75610500	1.66125000	3.75739300
H	-4.60610300	0.83660300	2.42557400
H	-7.72981700	-1.97768700	-3.27424000
H	-6.45459000	-3.16649900	-3.09436600
C	-7.96391600	-3.25158500	-1.55276100
H	-3.51386700	-3.70598300	-0.34020400
H	-4.98757700	-4.33951200	-1.10184100

H	-3.39345700	-4.76350200	-1.76619300
H	-8.56968400	-3.99813400	-2.08767900
H	-7.35634500	-3.78072400	-0.80346200
H	-8.64907700	-2.58016200	-1.01440000
C	-8.08894900	0.22910400	-1.28381300
S	-8.95795400	0.49623900	-2.77475000
C	-8.84348400	0.65891300	-0.21150400
C	-10.34075100	1.10305800	-1.94449900
C	-10.13806700	1.15423400	-0.59252600
O	-8.36261000	0.66295200	1.05630300
O	-11.04326200	1.69897300	0.26156000
C	-9.14274200	-0.04677400	2.04216300
C	-11.47584700	0.88448200	1.37168100
C	-10.38568000	0.74208900	2.42912100
H	-9.42070200	-1.02477800	1.61258100
C	-8.21665600	-0.26318800	3.22062100
C	-12.08706800	-0.42208200	0.89744600
H	-12.27236000	1.50049600	1.81264500
H	-10.06753900	1.74861700	2.74463800
H	-10.83996700	0.25864700	3.30913100
H	-8.72336300	-0.84474400	4.00285500
H	-7.31704100	-0.80911100	2.90698100
H	-7.90784200	0.70141800	3.65022300
H	-11.35208900	-1.07315700	0.40302200
H	-12.50858000	-0.97115800	1.75155000
H	-12.89740900	-0.22196400	0.18258600
C	8.83974200	-0.48345100	-0.52644200
C	9.62668200	-0.99249900	0.49613300
S	9.78824100	-0.18842900	-1.96105900
C	11.00163700	-1.14584800	0.10243200
C	9.12420100	-1.30428100	1.88320500
C	11.21750900	-0.75191400	-1.19397400
C	12.10651200	-1.65464500	0.98860300
H	8.26672800	-1.99238600	1.83307200
H	9.90574900	-1.85309400	2.42778700
C	8.72586900	-0.06230800	2.68103600
H	12.16063000	-0.75277800	-1.73692800
H	11.75589600	-2.53635800	1.54940700
H	12.92825800	-2.01108800	0.34931900
C	12.64768800	-0.61009400	1.96476400
H	8.39547400	-0.33921500	3.69317800
H	9.57055800	0.63603800	2.77752900
H	7.90122300	0.47604300	2.19114300
H	13.03794500	0.26568600	1.42481300
H	11.86815400	-0.25533600	2.65508300
H	13.46536900	-1.02892200	2.57014700

H	-11.22861200	1.41630900	-2.48674600
b. Radical Cation			
C	0.97796900	-0.88260200	0.16966700
C	1.62757500	-2.11502300	0.44316700
C	3.02791200	-2.02520600	0.37950700
C	3.48845400	-0.71849400	0.06983400
S	2.14668200	0.38949700	-0.11459100
C	4.81539800	-0.24535400	-0.13499500
C	5.20855800	1.07579800	-0.41462200
S	6.23276000	-1.27740400	-0.15153500
C	6.59408000	1.22834500	-0.63772900
C	7.31688900	0.04051400	-0.49997700
C	0.90267400	-3.37255500	0.83445400
H	0.07895400	-3.56905200	0.13279900
H	1.57673200	-4.22953300	0.71548400
C	3.93565100	-3.19352600	0.64543600
H	3.40018600	-4.12413900	0.41730700
H	4.77415700	-3.18288900	-0.06509000
C	4.45932300	-3.25212000	2.08215100
H	5.01913300	-2.34368100	2.34745400
H	3.63263600	-3.35771200	2.79893200
H	5.13074000	-4.11334100	2.20875500
C	0.37831900	-3.34803300	2.27277700
H	-0.14266900	-4.28816700	2.50320200
H	1.20342000	-3.23111900	2.98963800
H	-0.32753700	-2.52116300	2.43574600
O	4.29858700	2.05818700	-0.51783500
O	7.19097600	2.36734800	-1.04760400
C	4.51141100	3.28787800	0.23439300
C	7.04453100	3.54997000	-0.22229500
C	5.64208700	4.11774600	-0.35476500
H	7.25563100	3.25766200	0.81949300
H	5.43618100	4.29568900	-1.42172600
H	5.61859500	5.09939600	0.14431100
C	8.10181900	4.52083400	-0.70037400
H	8.07021200	5.43714300	-0.09561500
H	9.10176200	4.07779100	-0.61075500
H	7.92928400	4.79201300	-1.75209900
C	4.62159600	2.99767000	1.71924800
H	5.50785800	2.39561300	1.96477500
H	4.68921000	3.94289700	2.27588400
H	3.73379300	2.45404500	2.06976400
H	3.57514600	3.82667000	0.04173900
C	-0.40736700	-0.59772900	0.04751100
S	-1.63365600	-1.84104800	-0.09930200
C	-1.01409800	0.66977500	-0.07554900

C	-2.92708400	-0.68815700	-0.30554700
C	-2.40694500	0.61747300	-0.25943800
O	-0.27055300	1.78846600	-0.08252300
C	-4.28864600	-1.06031000	-0.53719600
O	-3.20581800	1.67611200	-0.49430500
C	-0.64397700	2.87250700	0.81382600
C	-4.87473200	-2.33428500	-0.67005900
S	-5.50273900	0.19141200	-0.70938300
C	-3.19543200	2.79040600	0.43717400
C	-1.89833600	3.57662600	0.32772000
H	-0.80418000	2.42883600	1.80963100
C	0.55187300	3.79574300	0.85750600
C	-6.27755000	-2.28006500	-0.89040500
C	-4.12903600	-3.63580400	-0.57420200
C	-6.76102800	-0.97222600	-0.93706300
C	-3.56604900	2.33966700	1.83729600
H	-4.00138600	3.42089300	0.03941300
H	-1.74873100	3.88147200	-0.71970500
H	-2.01968800	4.49913200	0.91680800
H	0.35641600	4.62606500	1.54907900
H	1.43943100	3.25449400	1.20710700
H	0.75638600	4.21264400	-0.13922500
C	-7.16746600	-3.49225800	-0.98614700
H	-4.62452700	-4.37339200	-1.22097800
H	-3.12242900	-3.52615100	-1.00233600
C	-4.04104200	-4.19070400	0.84925200
H	-2.83838200	1.63082700	2.25771800
H	-3.61497500	3.21101000	2.50552700
H	-4.55107700	1.85526500	1.83144500
H	-7.78271700	-3.43483400	-1.89610000
H	-6.54969000	-4.39125100	-1.10936000
C	-8.07799000	-3.66856700	0.23005500
H	-3.53367400	-3.48805600	1.52642700
H	-5.04271200	-4.38418300	1.25913500
H	-3.48128500	-5.13702800	0.85920300
H	-8.69372100	-4.57305700	0.12063600
H	-7.49172100	-3.76573800	1.15576300
H	-8.75497800	-2.81019200	0.34971200
C	-8.10849800	-0.49526000	-1.18762600
S	-9.10580000	-1.16278700	-2.45689000
C	-8.75946500	0.56588600	-0.57955400
C	-10.38894600	-0.06826600	-2.11822000
C	-10.07049500	0.80304700	-1.11150800
O	-8.17676400	1.31768000	0.38101000
O	-10.88113200	1.82823500	-0.74989000
C	-8.89578100	1.42913600	1.63317200

C	-11.24688600	1.92567600	0.64421200
C	-10.07348400	2.38379900	1.50436100
H	-9.24082000	0.41824100	1.90947800
C	-7.88079000	1.90782900	2.64858600
C	-11.94413200	0.66477100	1.12246100
H	-11.97811800	2.74588900	0.63321700
H	-9.69776900	3.34094500	1.10898400
H	-10.46306000	2.58539200	2.51509000
H	-8.34132400	1.97383500	3.64360700
H	-7.03405400	1.21114700	2.70246700
H	-7.50080100	2.90319200	2.37497700
H	-11.28014100	-0.21158600	1.11063100
H	-12.30660400	0.80360200	2.15091300
H	-12.80770200	0.44416100	0.47969200
C	8.73063900	-0.15154000	-0.69673500
C	9.55232400	-1.23064600	-0.35017000
S	9.64645200	1.07854000	-1.54757900
C	10.90128100	-1.05233200	-0.79398200
C	9.12143400	-2.43417800	0.44421900
C	11.07342700	0.14120400	-1.45446900
C	12.03156800	-2.02301400	-0.58169300
H	8.20827200	-2.87390300	0.01425900
H	9.88792700	-3.21403600	0.33546800
C	8.90911100	-2.14445700	1.93226500
H	11.99368900	0.52014600	-1.89544000
H	11.67708600	-3.05076500	-0.75960900
H	12.79593000	-1.83173000	-1.34957900
C	12.67692600	-1.93279600	0.80069200
H	8.61673500	-3.06148000	2.46409000
H	9.82982900	-1.76108700	2.39504700
H	8.11978700	-1.39563700	2.09052400
H	13.06325800	-0.91985500	0.98818000
H	11.96205500	-2.17156100	1.60143900
H	13.51712900	-2.63795500	0.88170400
H	-11.30808600	-0.09219300	-2.69716200