Electronic Supplementary Information: Photo-induced 6π-electrocyclisation and cycloreversion of isolated dithienylethene anions

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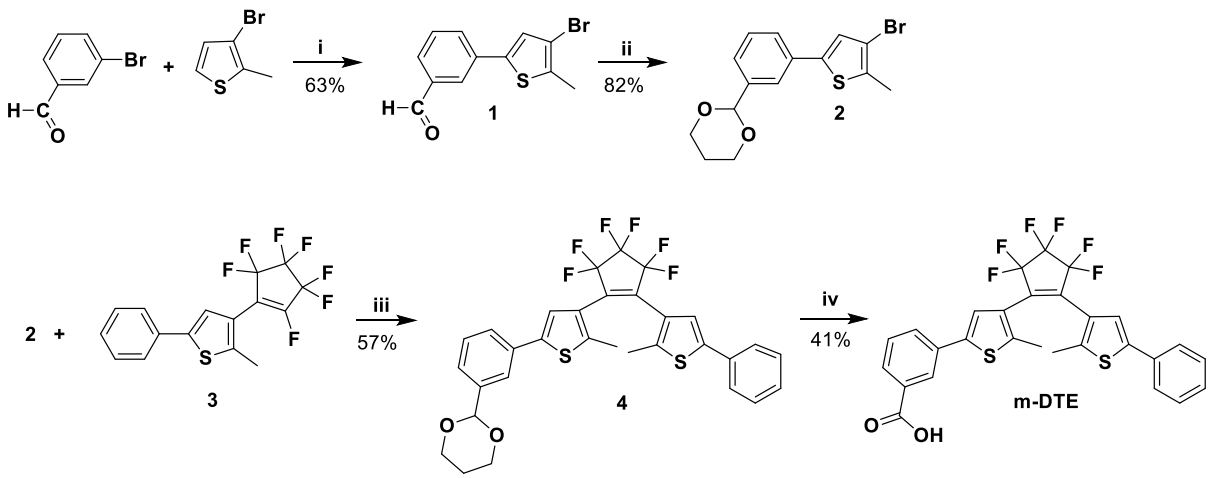
S1 Synthesis of *m*-DTE

S1.1 Materials. 3-bromobenzaldehyde (Sigma Aldrich) and 3-bromo-2-methylthiophene (Combi Blocks), palladium acetate (Sigma Aldrich), potassium carbonate (Univar), pivalic acid (Sigma Aldrich), dimethylacetamide (Sigma Aldrich), propandiol (Sigma Aldrich), *p*-toluenesulfonic acid (Sigma Aldrich), toluene (Univar), *n*-butyllithium (Sigma Aldrich), tetrahydrofuran (Unichrome), octafluorocyclopentene (Synquest Labs), chloroform-d (Sigma Aldrich) and sodium sulfate (Univar) were used as received. The preparation of *p*-DTE[1] and **3**[2] were previously reported.

S1.2 Characterisation. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AscendTM 400 MHz spectrometer or a Varian 300 MHz. Chemical shifts are reported in parts per million (ppm) and are referenced to the residual solvent peak (chloroform, ^{1}H=7.26 ppm and ^{13}C=77 ppm). Coupling constants (J) are quoted in Hertz (Hz) and quoted to the nearest 0.5 Hz. Peak multiplicities are described in the following manner: singlet (s), doublet (d), multiplet (m). Infrared spectra of the neat materials were recorded using a Shimadzu FTIR Spirit spectrometer equipped with an attenuated total reflection (ATR) crystal.



Scheme 1: Synthetic route to carboxylate functionalised *m*-DTE. Reagents and conditions: (i) $Pd(OAc)_2$, K_2CO_3, pivalic acid, dimethylacetamide, 100°C, Ar, 18 h. (ii) 1,3-propandiol, *p*-toluenesulfonic acid, toluene, reflux, overnight. (iii) **3**, *n*-butyllithium (1.45 M), tetrahydrofuran, -78°C; then **2**, -78°C to room temperature overnight. (iv) acetone, Jones reagent, 5 h.

S1.3 Synthetic Methodology.

3-(4-Bromo-5-methyl-thiophen-2-yl)-benzaldehyde (1):[3] A stirred solution of 2-methyl-3-bromothiophene (3.54 g, 20 mmol), 3-bromobenzaldehyde (3.70 g, 20 mmol), pivalic acid (0.80 g, 8 mmol) and potassium carbonate (6.60 g, 48 mmol) in dimethylacetamide (40 cm^3) was purged with argon for 20 min. To this solution palladium acetate (0.122 g, 4 mol%) was added prior to purging for a further 5 min. The reaction mixture was heated at 90°C for 18 h then allowed to cool to room temperature. Water (200 cm^3) was added to the reaction mixture prior to extracting with diethyl ether (2 x 150 cm^3). The combined ether extract was washed with brine (2 x 100 cm^3) and dried over Na_2SO_4 prior to the removal of the solvent. The product was purified by column chromatography over silica gel with a 1:1 mixture of petroleum ether / dichloromethane as eluent to afford the product as a white solid (3.54 g, 63 %). ν_{max} (neat)/cm^{-1}: 2838, 2744, 1686, 1599, 1580, 1490, 1434, 1386, 1287, 1251, 1155, 1082, 872, 785, 651; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 2.49 (s, 3H), 7.31 (s, 1H), 7.60 (t, J=7.7 Hz, 1H), 7.79-7.85 (m, 2H), 8.05 (m, 1H), 10.10 (s, 1H).

3-Bromo-5-(3-(2,6-dioxolanyl)phenyl)-2-methylthiophene (2): A stirred solution of **1** (3.59 g, 12.6 mmol), 1,3-propandiol (1.92 g, 25.0 mmol) and *p*-TsOH (0.11 g, 5 mol%) in toluene (40 cm^3) was heated at reflux overnight using a Dean Stark apparatus. The toluene was then removed under reduced pressure and the resulting residue taken up in diethyl ether (120 cm^3). The ether solution was washed with water (50 cm^3) and brine (50 cm^3) prior to drying over Na_2SO_4 and removal of the solvent under vacuum. The product was purified with column chromatography on silica gel by elution with DCM / petroleum ether (3:1) to afford **2** as a white solid (3.5 g, 82 %). ν_{max} (neat)/cm^{-1}: 2968, 2850, 1609, 1540, 1493, 1376, 1030, 955, 872, 730; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.43-1.50 (m, 1H), 2.16-2.33 (m, 1H), 2.41 (s, 3H), 3.96-4.05 (m, 2H), 4.26-4.32 (m, 2H), 5.52 (s, 1H), 7.13 (s, 1H), 7.33-7.41 (m, 2H), 7.45-7.49 (m, 1H), 7.64-7.65 (m, 1H).

1-(2-methyl-5-phenylthiophen-3-yl)-2-(5-(3-(2,6-dioxolanyl)phenyl)-2-methylthiophen-3-yl)perfluorocyclopentene (4): *n*-Butyllithium (1.52 cm^3, 1.45 M) was added dropwise to a stirred solution of **3** (0.75 g, 2.20 mmol) in dry THF (20 cm^3) at -78°C. The reaction was allowed to stir for 30 minutes prior to the dropwise addition of **2** (0.75 g, 2.42 mmol) in THF (2 cm^3). This reaction mixture was allowed to stir for 2 h at -78°C prior to slowly warming to room temperature overnight. The THF was removed under vacuum and the resulting residue taken up in diethyl ether (200 cm^3). This ether solution was consecutively washed with water (100 cm^3) and brine (100 cm^3) prior to drying over Na_2SO_4 and the removal of the solvent under vacuum. The product was purified by column chromatography on silica gel eluting with petroleum ether / DCM (3:2) to afford the product as a pale blue solid (704 mg, 57 %). ν_{max} (neat)/cm^{-1}: 2850, 1701, 1436, 1376, 1268, 1100, 985, 789, 688; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.43-1.51 (m, 1H), 1.95 (s, 6H), 2.17-2.31 (m, 1H), 3.96-4.05 (m, 2H), 4.26-4.32 (m, 2H), 5.53 (s, 1H), 7.28-7.43 (m, 7H), 7.48-7.56 (m, 3H), 7.67-7.68 (m, 1H).

1-(2-methyl-5-phenylthiophen-3-yl)-2-(5-(4-carboxylylphenyl)-2-methylthiophen-3-yl)perfluorocyclopentene (*m*-DTE): To a solution of **4** (0.41 g, 0.75 mmol) in acetone (20 cm^3), Jones reagent* (5.5 cm^3, 2.2 mmol) was added dropwise to a stirred solution at room temperature. The reaction was allowed to stir for 5 h prior to being quenched by the addition of propan-2-ol (2 cm^3). The acetone was then removed under vacuum and the aqueous residue taken up in diethyl ether (150 cm^3). The organic solution was then washed with water (2 x 100 cm^3) prior to drying over Na_2SO_4 and the removal of the solvent under vacuum. The product was purified by column chromatography on silica gel eluting with dichloromethane:tetrahydrofuran (9:1) to afford the product as a pale blue solid (175 mg, 41 %). ν_{max} (neat)/cm^{-1}: 2970, 2850, 1688, 1461, 1230, 1136, 990, 891, 814, 753; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.99 (s, 3H), 2.00 (s, 3H), 7.28-7.32 (m, 2H), 7.37-7.41 (m, 3H), 7.49-7.56 (m, 3H), 7.77-7.79 (m, 1H), 8.03-8.05 (m, 1H), 8.27 (m, 1H);

*** Jones Reagent Preparation:** A 3:1 ratio with respect to $[H^+]$ and $[Cr_2O_7^{2-}]$ was prepared in the following manner. To a solution of potassium dichromate (2.94 g, 10 mmol) in distilled water (20 cm^3) concentrated sulfuric acid (2.94 g; 1.6 cm^3; 30 mmol) was carefully added while keeping the temperature at room temperature or below. This solution was transferred quantitatively to a volumetric flask (25 cm^3) and made up to 25 cm^3 with distilled water.

S2 Photoaction spectra of *p*-DTE$^-$ and *m*-DTE$^-$

Figure S1: Left Column: Photoaction spectra for ring-closed *p*-DTE$^-$, measured by monitoring: (a) total photoproducts, (b) formation of ring-open *p*-DTE$^-$, (c) photofragment corresponding to CO_2 loss and (d) photofragment corresponding to F-atom loss.
Right Column: Photoaction spectra for ring-open *p*-DTE$^-$, measured by monitoring: (e) total photoproducts, (f) formation of ring-closed *p*-DTE$^-$ and (g) photofragment corresponding to CO_2 loss. The spectra are normalised with respect to laser power.

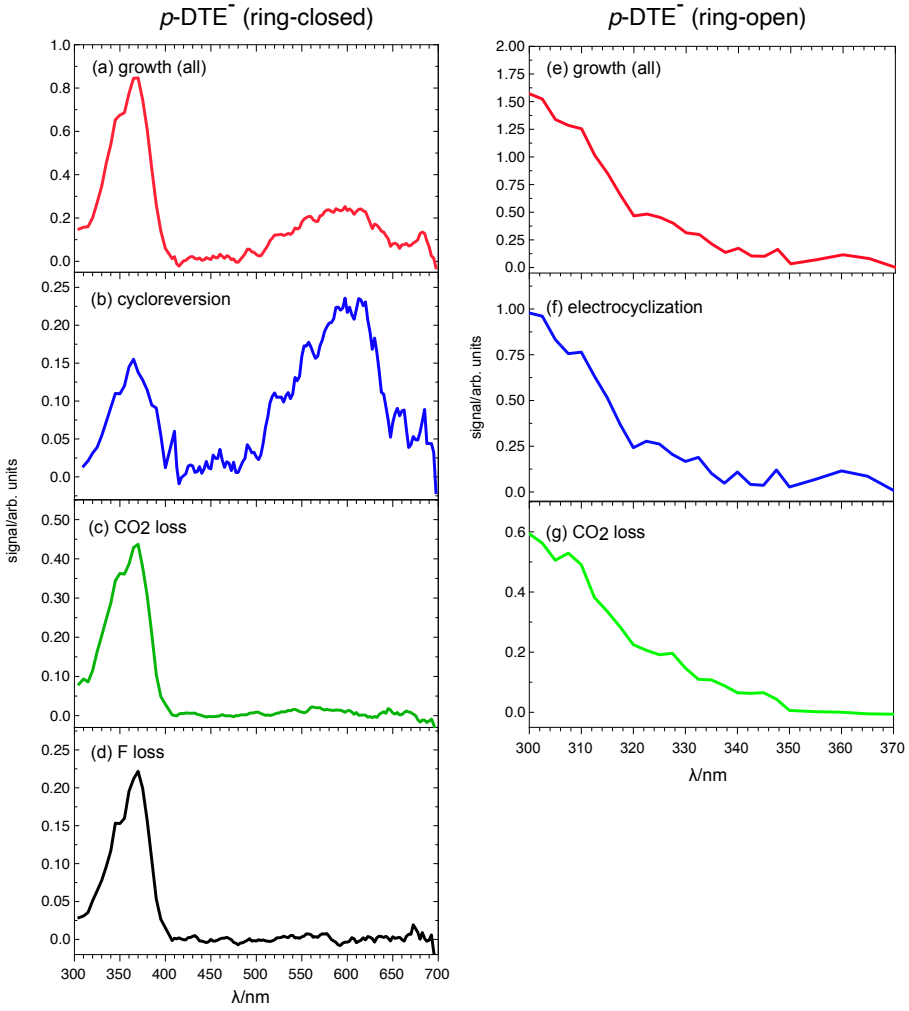
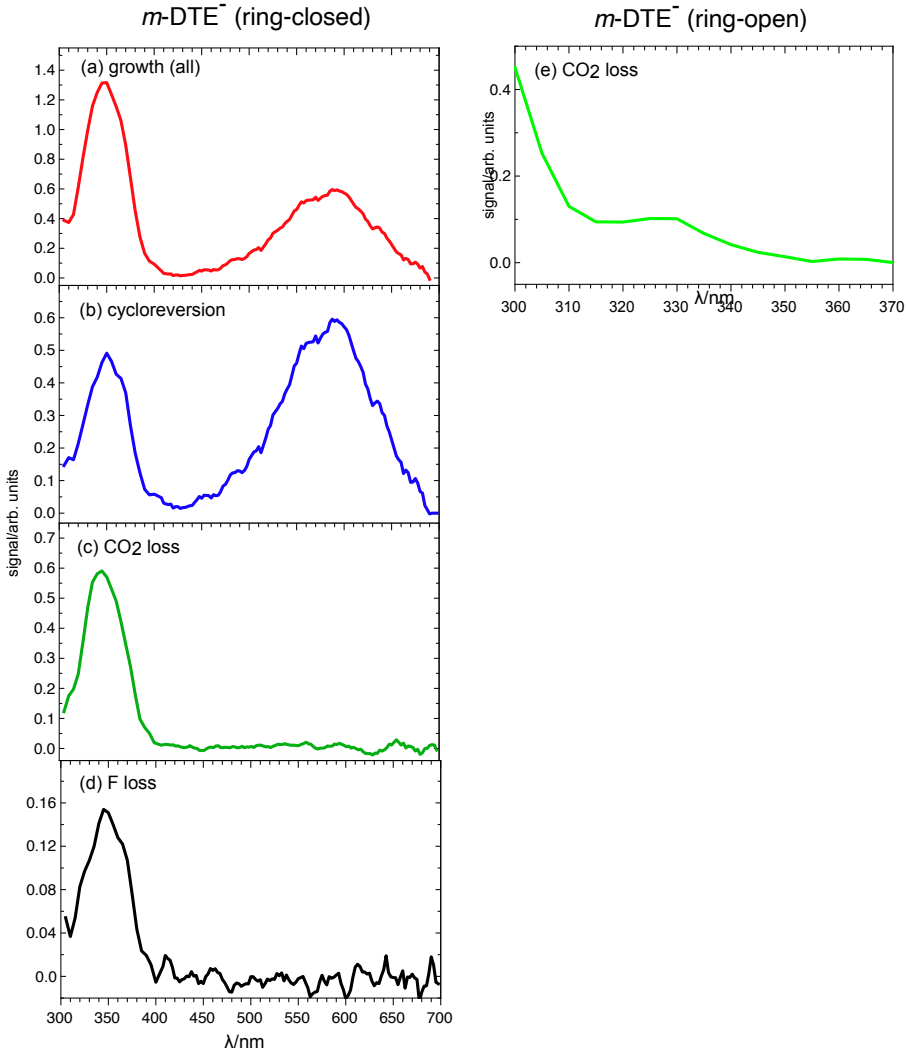
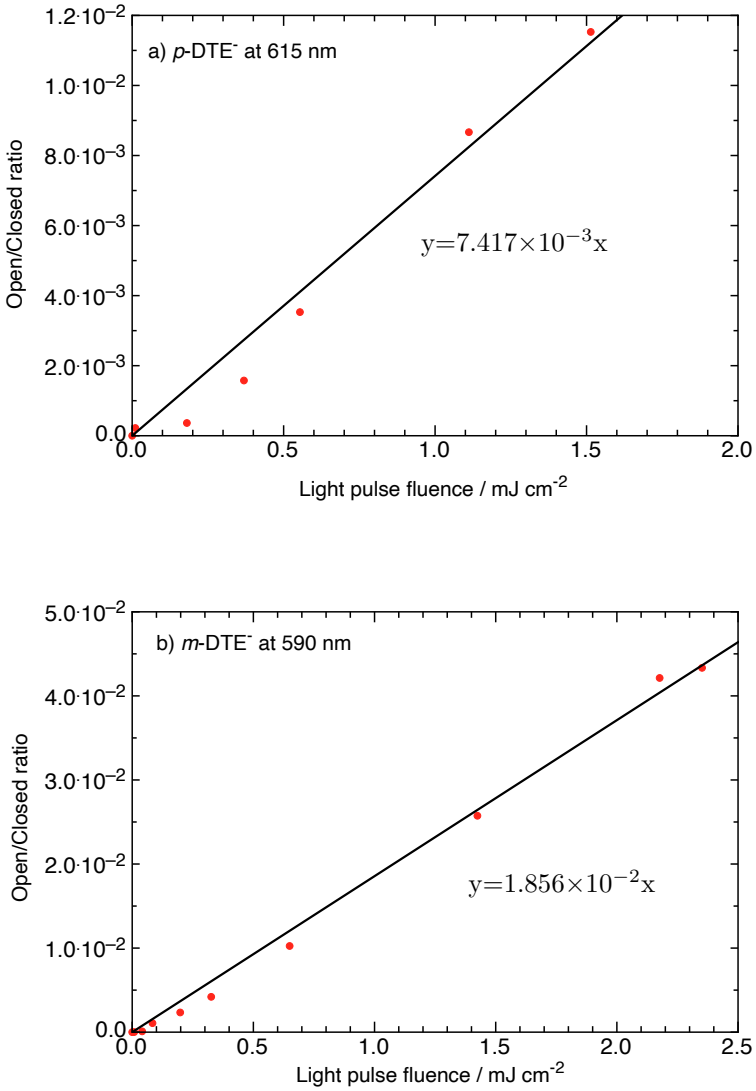


Figure S2: Left Column: Photoaction spectra for ring-closed m-DTE$^-$, measured by monitoring: (a) total photoproducts, (b) formation of ring-open m-DTE$^-$, (c) photofragment corresponding to CO_2 loss and (d) photofragment corresponding to F-atom loss.
Right Column: (e) Photoaction spectrum for ring-open m-DTE$^-$, measured by monitoring photofragment signal corresponding to CO_2 loss. The spectra are normalised with respect to laser power.



S3 Isomerisation yields with light pulse fluence

Figure S3: Measured photoisomerisation yield ratios as a function of light pulse fluence for the cycloreversion reaction of a) *p*-DTE$^-$ at 615 nm (peak of first PISA band) and b) *m*-DTE$^-$ at 590 nm (peak of first PISA band).

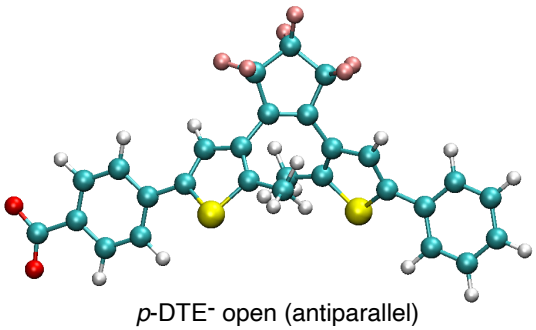


S4 Computational Methods

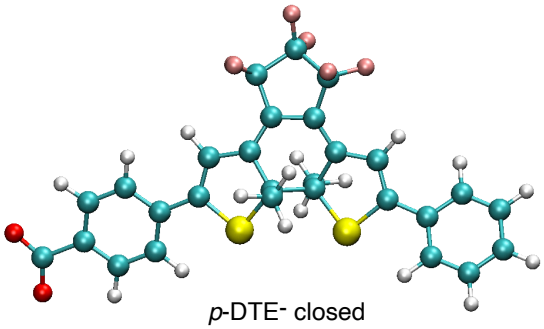
Density functional theory (DFT) calculations for the *p*-DTE and *m*-DTE anions were performed using the Gaussian 16 software suite.[4] Geometry optimizations, harmonic vibrational frequencies and transition-state structures for the DTE anions were calculated using the dispersion-corrected DFT functional ωB97X-D and the aug-cc-pVDZ basis set. Calculated electronic energies were corrected for vibrational zero-point energy and used for constructing the potential energy surfaces shown in Fig. 1 in the main text. Adiabatic electron affinities for the DTE photoswitch isomers were computed at the ωB97X-D/aug-cc-pVDZ level of theory. Vertical excitation energies and oscillator strengths were calculated using time-dependent density functional theory (TD-DFT) at the ωB97X-D/aug-cc-pVDZ level of theory.

S5 Gas-phase molecular structures

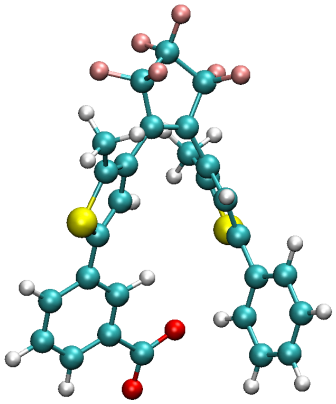
Figure S4: Optimised gas-phase structures for *p*-DTE$^-$ and *m*-DTE$^-$ molecules at the ωB97X-D/aug-cc-pVDZ level of theory. Only the lowest energy ring-open structures are displayed.



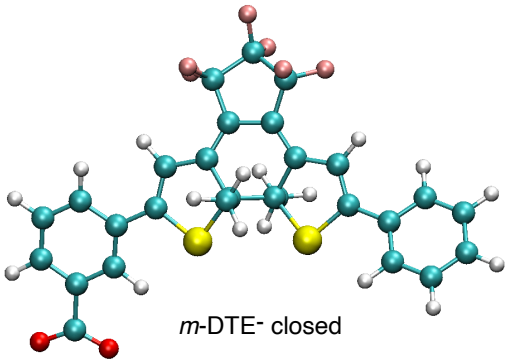
p-DTE$^-$ open (antiparallel)



p-DTE$^-$ closed



m-DTE$^-$ open (parallel)



m-DTE$^-$ closed

S6 Cartesian coordinates

Table S1: Atomic Cartesian coordinates for the antiparallel *p*-DTE^{-} structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.00981	-2.28581	0.0432
C	-4.68506	-1.99011	0.35202
C	-4.23599	-0.66118	0.36588
C	-5.15242	0.3595	0.0692
C	-6.47312	0.05224	-0.24401
C	-6.92159	-1.27195	-0.26263
H	-6.37581	-3.31232	0.02214
H	-3.98468	-2.8013	0.56301
H	-4.82905	1.40128	0.10639
H	-7.20035	0.83094	-0.47401
C	-8.39464	-1.60844	-0.61157
O	-9.11807	-0.62045	-0.86912
O	-8.67896	-2.82714	-0.59375
C	-2.83611	-0.32917	0.66474
C	-2.08009	0.71302	0.20393
S	-1.87895	-1.31753	1.74249
C	-0.72563	0.70043	0.67839
H	-2.46212	1.44471	-0.50222
C	-0.45975	-0.34618	1.53143
C	0.28897	1.67009	0.25833
C	1.53044	1.4206	-0.21405
C	2.14641	0.12857	-0.53249
C	3.46567	-0.2234	-0.09667
C	3.84803	-1.4827	-0.46116
H	4.08548	0.43206	0.5103
S	2.5813	-2.24656	-1.38356
C	1.53599	-0.86951	-1.25678
C	5.11439	-2.17146	-0.1667
C	5.17015	-3.56286	-0.00534
C	6.29962	-1.43288	-0.0351
C	6.3758	-4.19695	0.28381

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Table S1 – *Continued from previous page*

Atom	Coordinates		
H	4.25742	-4.15351	-0.08875
C	7.50166	-2.06735	0.26436
H	6.27944	-0.35397	-0.18715
C	7.54629	-3.45254	0.4234
H	6.39827	-5.27969	0.40843
H	8.41264	-1.47653	0.36202
H	8.48915	-3.94917	0.65236
C	0.06287	3.15413	0.41742
C	1.25397	3.81466	-0.32504
C	2.32119	2.69198	-0.35978
F	1.68941	4.94144	0.2658
F	0.8872	4.11615	-1.591
F	3.06149	2.74254	-1.49355
F	3.19869	2.86291	0.67994
F	0.08488	3.51147	1.73189
F	-1.11962	3.58487	-0.08498
C	0.80896	-0.69478	2.24605
H	1.38171	-1.45945	1.70145
H	1.44675	0.19153	2.34767
H	0.59929	-1.0794	3.25157
C	0.18929	-0.8901	-1.90748
H	-0.56541	-1.34187	-1.24919
H	-0.13877	0.13105	-2.13283
H	0.21307	-1.4597	-2.84389

Table S2: Atomic Cartesian coordinates for the parallel *p*-DTE$^-$ structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-4.42558	1.70485	0.08008
C	-3.11683	2.1006	0.33736
C	-2.11258	1.89379	-0.618
C	-2.46949	1.35394	-1.86249
C	-3.78754	0.98685	-2.11972
C	-4.77473	1.11713	-1.13799
H	-5.19669	1.78682	0.84525
H	-2.85576	2.50231	1.31791
H	-1.70262	1.21193	-2.62576
C	-0.69563	2.08075	-0.27077
C	0.33598	1.25122	-0.59151
S	-0.12781	3.31763	0.81822
C	1.57154	1.54585	0.07962
H	0.19349	0.39487	-1.2414
C	1.48079	2.67313	0.8718
C	2.70214	0.60846	0.02634
C	4.15191	1.01704	0.1187
C	3.96545	-1.3842	-0.105
C	2.60827	-0.73868	-0.09979
F	4.26752	-1.92479	1.11313
F	4.10715	-2.38843	-1.00708
F	4.55271	1.2512	1.40579
F	4.44945	2.13316	-0.59101
C	1.3521	-1.50995	-0.14603
C	0.37256	-1.42365	0.89766
C	-0.8351	-1.96361	0.5614
H	0.53942	-0.88934	1.83001
S	-0.76037	-2.63958	-1.04221
C	0.89045	-2.15939	-1.26542
C	-2.09836	-1.93354	1.32105
C	-2.11933	-2.28343	2.67752
C	-3.27878	-1.4934	0.70831
C	-3.30536	-2.19027	3.40207

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Table S2 – *Continued from previous page*

Atom	Coordinates		
H	-1.20572	-2.63734	3.15654
C	-4.46615	-1.39448	1.43212
H	-3.26397	-1.17372	-0.33399
C	-4.47558	-1.74738	2.78187
H	-3.31596	-2.467	4.45735
H	-5.36551	-1.00452	0.94339
H	-5.40003	-1.668	3.35456
C	2.49343	3.34278	1.75351
H	2.06147	4.23509	2.22153
H	2.8305	2.67137	2.5531
H	3.37618	3.65431	1.18242
C	1.56545	-2.36234	-2.58894
H	2.09231	-3.32437	-2.6311
H	2.30276	-1.56984	-2.76724
H	0.83548	-2.33702	-3.40708
C	4.92794	-0.21467	-0.41098
F	6.14531	-0.3554	0.14418
F	5.09028	-0.10357	-1.75098
C	-6.18928	0.53979	-1.36112
O	-6.81667	0.27458	-0.30479
O	-6.52724	0.37403	-2.55111
H	-4.08116	0.56431	-3.08051

Table S3: Atomic Cartesian coordinates for the closed anti-configured *p*-DTE$^-$ structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-5.89624	-2.24118	-0.32115
C	-4.53639	-1.96843	-0.24695
C	-4.07827	-0.67649	0.06866
C	-5.03405	0.32907	0.31511
C	-6.39023	0.04536	0.24324
C	-6.84224	-1.24077	-0.07698
H	-6.26947	-3.23431	-0.56957
H	-3.81906	-2.76618	-0.44853
H	-4.71152	1.3358	0.58122
H	-7.1453	0.80677	0.437
C	-8.36096	-1.55049	-0.15556
O	-9.10907	-0.57862	0.08726
O	-8.64211	-2.7323	-0.45147
C	-2.65339	-0.37835	0.13805
C	-2.05802	0.85473	0.19884
S	-1.48644	-1.71086	0.1316
C	-0.63805	0.83017	0.23095
H	-2.62273	1.78095	0.15132
C	-0.0771	-0.57004	0.48498
C	0.26886	1.83922	0.10301
C	1.69343	1.56227	0.04048
C	2.17413	0.31264	-0.14097
C	3.52524	-0.17828	-0.12541
C	3.62849	-1.52923	-0.0932
H	4.38518	0.48422	-0.07323
S	2.06361	-2.36813	-0.08023
C	1.14948	-0.7879	-0.42412
C	4.87201	-2.31398	-0.04304
C	4.88579	-3.61348	0.48293
C	6.07535	-1.77139	-0.52094
C	6.07039	-4.3429	0.546
H	3.9629	-4.05432	0.8601
C	7.25757	-2.50099	-0.45684

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Table S3 – *Continued from previous page*

Atom	Coordinates		
H	6.0806	-0.7769	-0.96554
C	7.2612	-3.78983	0.07863
H	6.06112	-5.3498	0.9632
H	8.18139	-2.06458	-0.83685
H	8.18774	-4.36218	0.12458
C	0.24936	-0.66875	1.99024
H	0.58177	-1.67809	2.25202
H	1.03799	0.04542	2.25764
H	-0.65137	-0.43095	2.56621
C	0.81032	-0.75037	-1.92725
H	1.73559	-0.84267	-2.50679
H	0.13596	-1.56802	-2.19952
H	0.3292	0.20224	-2.18138
C	0.02159	3.30795	0.06325
C	1.41378	3.91588	-0.29662
C	2.44433	2.84804	0.17581
F	2.78633	3.11191	1.47488
F	3.5938	2.92018	-0.545
F	1.62351	5.12872	0.24373
F	1.50921	4.03231	-1.64366
F	-0.92141	3.70402	-0.83595
F	-0.38073	3.81273	1.27189

Table S4: Atomic Cartesian coordinates for the byproduct of *p*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	5.72340	-1.81770	0.80360
C	4.34320	-1.65010	0.76960
C	3.76510	-0.68340	-0.07140
C	4.61060	0.09060	-0.88660
C	5.98760	-0.09260	-0.84900
C	6.56450	-1.04590	-0.00320
H	3.70780	-2.25060	1.42110
H	4.17570	0.81680	-1.57480
H	6.65940	0.48890	-1.48030
C	2.31080	-0.45980	-0.11300
C	1.76170	0.78260	-0.25590
S	1.36370	-1.95990	0.01780
C	0.35520	1.01470	-0.36440
H	2.43420	1.63760	-0.21670
C	-0.60110	-0.13400	-0.63930
C	-0.41260	2.13080	-0.23590
C	-1.82270	1.77820	-0.25600
C	-1.98450	0.44280	-0.40640
C	-3.13460	-0.41490	-0.31440
C	-3.04490	-1.76070	-0.16230
H	-4.12480	0.03910	-0.28820
S	-1.51860	-2.66560	-0.03780
C	-0.33100	-1.28830	0.32890
C	-4.25640	-2.61250	-0.08600
C	-4.36010	-3.65770	0.84270
C	-5.33460	-2.36840	-0.94880
C	-5.52130	-4.42210	0.91990
H	-3.52990	-3.85930	1.51840
C	-6.49450	-3.13450	-0.86990
H	-5.25090	-1.58280	-1.69920
C	-6.59300	-4.16360	0.06590
H	-5.58950	-5.22440	1.65480
H	-7.32140	-2.93320	-1.55110

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Table S4 – *Continued from previous page*

Atom	Coordinates		
H	-7.49930	-4.76650	0.12500
C	-0.48190	-0.48810	-2.14140
H	-1.19970	-1.26750	-2.41630
H	-0.69570	0.41300	-2.72790
H	0.52870	-0.83270	-2.38100
C	-0.46040	-0.88350	1.80180
H	-1.47060	-0.51420	2.01760
H	-0.25740	-1.74920	2.44000
H	0.26220	-0.09520	2.04500
C	-0.23790	3.58230	0.03070
C	-1.63910	3.99760	0.60570
C	-2.66410	2.98240	-0.01020
F	-3.16610	3.51070	-1.16650
F	-3.72160	2.78550	0.81750
F	-1.95690	5.27900	0.35510
F	-1.62220	3.82130	1.94880
F	0.75540	3.89580	0.89770
F	-0.00570	4.30770	-1.10700
C	8.10260	-1.24620	0.03350
O	8.74980	-0.50320	-0.73680
O	8.50160	-2.12540	0.82860
H	6.19310	-2.55060	1.45940

Table S5: Atomic Cartesian coordinates for TS1 local maximum of *p*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-5.46214	-0.81984	0.70837
C	-4.18769	-0.51693	1.18039
C	-3.4344	0.50765	0.58918
C	-3.99831	1.22321	-0.47861
C	-5.26975	0.90699	-0.94773
C	-6.01963	-0.11869	-0.36425
H	-6.05951	-1.6166	1.15155
H	-3.76112	-1.0981	2.00076
H	-3.44115	2.04748	-0.92776
H	-5.72481	1.45247	-1.77454
C	-7.43436	-0.46855	-0.8939
O	-7.82476	0.22253	-1.86165
O	-8.01219	-1.40044	-0.29062
C	-2.07073	0.81767	1.04024
C	-1.01611	1.28255	0.30411
S	-1.57326	0.59946	2.69975
C	0.18688	1.45372	1.06047
H	-1.08201	1.47365	-0.76358
C	0.05188	1.12149	2.38358
C	1.4481	1.85926	0.41756
C	2.14655	1.11661	-0.45626
C	1.82902	-0.26545	-0.86086
C	2.26	-1.40503	-0.11276
C	1.80229	-2.5896	-0.61873
H	2.8545	-1.33194	0.79512
S	0.83605	-2.30403	-2.03994
C	1.04794	-0.58623	-1.9401
C	2.02987	-3.94774	-0.10037
C	1.03921	-4.93587	-0.1848
C	3.25261	-4.27051	0.50572
C	1.26543	-6.2114	0.32592
H	0.07422	-4.69673	-0.63222
C	3.47256	-5.54319	1.02514

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Table S5 – *Continued from previous page*

Atom	Coordinates		
H	4.04156	-3.52	0.55313
C	2.48097	-6.52009	0.93542
H	0.48105	-6.96508	0.25652
H	4.42927	-5.77685	1.493
H	2.6549	-7.51779	1.33855
C	2.10332	3.19973	0.63575
C	3.13685	3.31165	-0.52079
C	3.37075	1.83698	-0.94628
F	4.26737	3.94596	-0.16217
F	2.58152	3.98876	-1.55136
F	3.55481	1.73093	-2.28562
F	4.50514	1.35485	-0.35828
F	2.75565	3.25979	1.83419
F	1.22709	4.22875	0.61704
C	1.08789	1.12188	3.46666
H	0.94247	0.27689	4.15123
H	2.09225	1.04042	3.0336
H	1.05467	2.0469	4.05854
C	0.39424	0.33093	-2.926
H	-0.69677	0.206	-2.91902
H	0.62342	1.37366	-2.67657
H	0.75124	0.14229	-3.94649

Table S6: Atomic Cartesian coordinates for TS2 local maximum of *p*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-5.84075	-2.18633	0.23059
C	-4.49526	-1.93261	0.43285
C	-3.97351	-0.63155	0.26202
C	-4.85941	0.40038	-0.12044
C	-6.20533	0.13521	-0.31672
C	-6.71585	-1.15761	-0.14594
H	-6.2647	-3.18228	0.35452
H	-3.83258	-2.7499	0.7229
H	-4.49129	1.41622	-0.25931
H	-6.90792	0.91482	-0.60916
C	-8.22464	-1.44838	-0.36966
O	-8.90259	-0.45461	-0.70536
O	-8.55859	-2.63765	-0.18327
C	-2.57427	-0.35115	0.47752
C	-1.905	0.88129	0.27083
S	-1.45397	-1.55575	0.98908
C	-0.55377	0.82903	0.51478
H	-2.40831	1.77207	-0.09324
C	-0.04317	-0.47298	0.86579
C	0.42418	1.89197	0.21063
C	1.62569	1.58013	-0.37044
C	2.04181	0.26123	-0.70123
C	3.35019	-0.26472	-0.52051
C	3.44584	-1.6249	-0.45326
H	4.20793	0.38635	-0.36915
S	1.83547	-2.35648	-0.69182
C	1.00239	-0.77495	-0.77406
C	4.61182	-2.45701	-0.18312
C	4.49732	-3.84724	-0.00088
C	5.90216	-1.89532	-0.09391
C	5.61392	-4.63592	0.26701
H	3.51821	-4.32262	-0.06604
C	7.01295	-2.68515	0.17305

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Table S6 – *Continued from previous page*

Atom	Coordinates		
H	6.03816	-0.82422	-0.23851
C	6.88103	-4.06413	0.35744
H	5.48815	-5.71048	0.40499
H	7.9972	-2.21927	0.2355
H	7.75507	-4.68128	0.56493
C	0.95478	-0.64136	1.99356
H	1.30255	-1.68067	2.04463
H	1.82422	0.00169	1.82467
H	0.5015	-0.36995	2.95492
C	-0.01514	-0.70706	-1.9008
H	0.49889	-0.95686	-2.83517
H	-0.84203	-1.4139	-1.7634
H	-0.42049	0.30433	-2.0025
C	0.2289	3.33748	0.41521
C	1.64916	3.93566	0.21101
C	2.41563	2.84382	-0.59173
F	3.70956	2.76159	-0.17877
F	2.4501	3.17987	-1.90964
F	2.24219	4.10884	1.41608
F	1.6409	5.12644	-0.41727
F	-0.6479	3.91457	-0.48288
F	-0.27141	3.65789	1.64411

Table S7: Atomic Cartesian coordinates for TS3 local maximum of *p*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-5.94612	-1.77541	-0.61494
C	-4.56076	-1.83634	-0.55855
C	-3.83348	-0.92055	0.22459
C	-4.55342	0.03947	0.96479
C	-5.94151	0.07108	0.92544
C	-6.65884	-0.82583	0.12711
H	-4.01817	-2.58426	-1.13549
H	-4.02700	0.73869	1.61558
H	-6.51325	0.79115	1.51021
C	-2.36171	-0.97077	0.29173
C	-1.68802	0.29733	0.48278
S	-1.53391	-2.41762	0.04865
C	-0.34524	0.56033	0.48153
H	-2.33332	1.17445	0.46758
C	0.81553	-0.43033	0.46239
C	0.26304	1.85231	0.37784
C	1.62723	1.74477	0.20260
C	2.05721	0.40825	0.19965
C	3.33528	-0.19070	0.17698
C	3.50317	-1.50138	-0.18561
H	4.21501	0.39961	0.43518
S	2.18851	-2.27354	-1.07785
C	0.88507	-1.15869	-0.83759
C	4.74311	-2.27507	0.00709
C	5.13622	-3.28472	-0.88584
C	5.57507	-1.99724	1.10285
C	6.32642	-3.97986	-0.69687
H	4.51375	-3.52094	-1.74914
C	6.77321	-2.68393	1.28290
H	5.26602	-1.24878	1.83198
C	7.15422	-3.68013	0.38543
H	6.61289	-4.75792	-1.40463
H	7.40390	-2.45032	2.14092

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Table S7 – *Continued from previous page*

Atom	Coordinates		
H	8.08667	-4.22523	0.53182
C	0.92870	-1.19797	1.78603
H	1.72555	-1.94757	1.74161
H	1.17984	-0.47183	2.56968
H	-0.00948	-1.69475	2.03484
C	0.17394	-0.71723	-2.08266
H	0.68673	0.16338	-2.50076
H	0.21690	-1.50946	-2.83906
H	-0.86846	-0.45146	-1.89076
C	-0.20262	3.26302	0.33974
C	1.05312	4.03274	-0.20334
C	2.27092	3.08597	0.07279
F	2.89232	3.46208	1.22760
F	3.19643	3.16799	-0.91386
F	1.20508	5.24710	0.35217
F	0.92727	4.19513	-1.54034
F	-1.28248	3.48532	-0.45178
F	-0.52711	3.74326	1.57701
C	-8.20848	-0.77176	0.06996
O	-8.73195	0.11093	0.78480
O	-8.73824	-1.61793	-0.68323
H	-6.52279	-2.46248	-1.23377

Table S8: Atomic Cartesian coordinates for the *m*-DTE$^-$ structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.32919	-1.52304	-0.21679
C	-4.99265	-1.3294	0.13177
C	-4.4346	-0.0463	0.19678
C	-5.24085	1.06638	-0.08736
C	-6.57561	0.88025	-0.43922
C	-7.116	-0.40517	-0.50345
H	-4.40329	-2.22701	0.32874
H	-4.82785	2.07321	-0.01077
H	-7.20061	1.74905	-0.65454
C	-3.017	0.14908	0.53908
C	-2.15318	1.11731	0.10806
S	-2.19283	-0.93776	1.62803
C	-0.81974	0.96925	0.61674
H	-2.44285	1.88574	-0.60309
C	-0.68316	-0.10466	1.46771
C	0.29573	1.83395	0.22643
C	1.5196	1.46393	-0.21338
C	2.01536	0.11823	-0.5186
C	3.28614	-0.35656	-0.05608
C	3.55403	-1.64743	-0.41254
H	3.95323	0.23759	0.56381
S	2.23932	-2.28962	-1.35964
C	1.3273	-0.81964	-1.25458
C	4.74232	-2.45336	-0.09135
C	4.66125	-3.84344	0.07104
C	5.98984	-1.83139	0.06553
C	5.79439	-4.58934	0.38551
H	3.69819	-4.34428	-0.03151
C	7.11909	-2.57734	0.3904
H	6.07612	-0.75571	-0.0865
C	7.0276	-3.96015	0.55008
H	5.71016	-5.66898	0.51056
H	8.08016	-2.07616	0.50776

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Table S8 – *Continued from previous page*

Atom	Coordinates		
H	7.91348	-4.54434	0.79915
C	0.21128	3.33295	0.37977
C	1.48011	3.87297	-0.32966
C	2.43376	2.65215	-0.33559
F	2.00648	4.95442	0.27287
F	1.17877	4.20684	-1.60516
F	3.20708	2.62997	-1.44833
F	3.29471	2.74089	0.72816
F	0.23105	3.69159	1.69417
F	-0.90986	3.87758	-0.15492
C	0.52516	-0.58094	2.21299
H	1.02704	-1.40307	1.6826
H	1.24965	0.23393	2.33004
H	0.25183	-0.94017	3.21255
C	-0.00238	-0.7163	-1.93181
H	-0.80917	-1.08801	-1.28539
H	-0.2257	0.32967	-2.17127
H	-0.01624	-1.29536	-2.8625
C	-6.91813	-2.95647	-0.29203
O	-8.12839	-3.01814	-0.60196
O	-6.10874	-3.876	-0.03411
H	-8.15768	-0.57957	-0.77307

Table S9: Atomic Cartesian coordinates for the parallel *m*-DTE$^-$ structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-4.06325	3.88844	-0.56117
C	-2.75053	3.7555	-0.11165
C	-2.10607	2.51451	-0.19818
C	-2.80099	1.42083	-0.73471
C	-4.11048	1.54821	-1.19502
C	-4.73775	2.7938	-1.10084
H	-4.55925	4.85843	-0.49358
H	-2.22066	4.62134	0.2899
H	-2.34079	0.4342	-0.79107
C	-0.72006	2.3297	0.26153
C	0.20851	1.45046	-0.20858
S	-0.05094	3.22023	1.60376
C	1.45642	1.46517	0.50393
H	0.00801	0.80532	-1.05794
C	1.47356	2.40129	1.51683
C	2.53086	0.5215	0.16928
C	4.0011	0.84261	0.27173
C	3.68211	-1.40427	-0.56962
C	2.36192	-0.73872	-0.29744
F	4.02371	-2.26984	0.43135
F	3.71886	-2.12423	-1.71928
F	4.47966	0.71666	1.54852
F	4.31858	2.09544	-0.13891
C	1.07724	-1.44417	-0.43639
C	0.21468	-1.66572	0.68278
C	-1.0092	-2.16747	0.33579
H	0.48112	-1.39923	1.70295
S	-1.10902	-2.37531	-1.38817
C	0.50201	-1.79507	-1.63519
C	-2.14981	-2.47209	1.2162
C	-1.92184	-3.01159	2.4905
C	-3.46202	-2.19917	0.80483
C	-2.98821	-3.26442	3.3492

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Table S9 – *Continued from previous page*

Atom	Coordinates		
H	-0.90333	-3.24668	2.80177
C	-4.52331	-2.46013	1.67006
H	-3.66651	-1.74556	-0.17472
C	-4.29421	-2.98947	2.93988
H	-2.79992	-3.68548	4.33775
H	-5.5369	-2.23087	1.34096
H	-5.13041	-3.18755	3.61181
C	2.53863	2.75008	2.51447
H	2.16591	3.49436	3.22802
H	2.85504	1.86607	3.0812
H	3.4257	3.16832	2.02256
C	1.0385	-1.61805	-3.02429
H	1.50051	-2.54044	-3.39992
H	1.80174	-0.83034	-3.04208
H	0.2369	-1.33141	-3.71583
C	4.68686	-0.23069	-0.61023
F	5.92094	-0.55905	-0.18427
F	4.79298	0.23	-1.87911
C	-4.86288	0.33164	-1.78421
O	-6.03291	0.54706	-2.15692
O	-4.20673	-0.74167	-1.81968
H	-5.7637	2.87069	-1.46008

Table S10: Atomic Cartesian coordinates for the closed anti-configured *m*-DTE$^-$ structure calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.24899	-1.41445	-0.14402
C	-4.86422	-1.26628	-0.09566
C	-4.27009	-0.03707	0.2298
C	-5.09673	1.06455	0.52318
C	-6.47753	0.92195	0.48183
C	-7.04966	-0.30938	0.14806
H	-4.27475	-2.15283	-0.33864
H	-4.66105	2.02347	0.80258
H	-7.11399	1.77622	0.71803
C	-2.81602	0.10778	0.26281
C	-2.0958	1.27317	0.27065
S	-1.80627	-1.34132	0.27968
C	-0.68553	1.09769	0.27465
H	-2.56064	2.25179	0.19627
C	-0.27426	-0.34677	0.56269
C	0.31957	1.99881	0.09172
C	1.70491	1.56817	0.00692
C	2.04324	0.2686	-0.14219
C	3.33391	-0.36421	-0.13971
C	3.29154	-1.71691	-0.06237
H	4.26088	0.20295	-0.12983
S	1.64809	-2.38153	0.01353
C	0.89949	-0.72379	-0.36397
C	4.44482	-2.62949	-0.01228
C	4.32899	-3.90941	0.5479
C	5.6897	-2.23235	-0.52541
C	5.42914	-4.76099	0.60967
H	3.37143	-4.23891	0.95139
C	6.7875	-3.08376	-0.46262
H	5.79307	-1.25558	-0.99658
C	6.66293	-4.35182	0.10705
H	5.3194	-5.75071	1.05283
H	7.74502	-2.75957	-0.87054

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Table S10 – *Continued from previous page*

Atom	Coordinates		
H	7.52299	-5.02003	0.15179
C	0.07693	-0.43305	2.06355
H	0.30482	-1.46398	2.35155
H	0.94372	0.19981	2.29119
H	-0.77931	-0.08271	2.64992
C	0.52772	-0.69958	-1.85991
H	1.42267	-0.90963	-2.45615
H	-0.23669	-1.44856	-2.08806
H	0.14447	0.29038	-2.13689
C	0.22971	3.48289	0.00506
C	1.66913	3.92544	-0.40614
C	2.59156	2.76901	0.08102
F	2.9925	3.03863	1.36259
F	3.72416	2.6952	-0.66601
F	2.02037	5.12644	0.08665
F	1.74205	3.98811	-1.75812
F	-0.68843	3.95	-0.88693
F	-0.08649	4.06953	1.20332
H	-8.13	-0.45087	0.10801
C	-6.88044	-2.78273	-0.51472
O	-8.13042	-2.80376	-0.51384
O	-6.05805	-3.69037	-0.76707

Table S11: Atomic Cartesian coordinates for the byproduct of *m*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.10270	-0.90800	0.05670
C	-4.71170	-0.93160	0.15330
C	-3.93380	0.14520	-0.29510
C	-4.56850	1.25820	-0.87070
C	-5.95570	1.28160	-0.97890
C	-6.71740	0.20710	-0.51560
H	-4.27160	-1.81350	0.62220
H	-3.97550	2.08620	-1.26010
H	-6.44370	2.14290	-1.43820
C	-2.46260	0.12690	-0.16030
C	-1.74090	1.24070	0.15070
S	-1.76100	-1.47590	-0.47700
C	-0.32020	1.23320	0.32150
H	-2.28220	2.17630	0.28060
C	0.41990	-0.07990	0.51160
C	0.62010	2.21420	0.35940
C	1.95310	1.63420	0.41410
C	1.88940	0.28270	0.42120
C	2.89060	-0.74600	0.33120
C	2.59810	-2.03370	0.02380
H	3.93190	-0.48320	0.51580
S	0.97240	-2.64840	-0.35970
C	0.03960	-1.06080	-0.59780
C	3.65060	-3.07830	-0.03270
C	3.43180	-4.35460	0.50310
C	4.89040	-2.79880	-0.62390
C	4.43490	-5.32000	0.46460
H	2.47510	-4.58870	0.97000
C	5.89160	-3.76560	-0.66160
H	5.06150	-1.82210	-1.07570
C	5.66860	-5.02950	-0.11610
H	4.25030	-6.30480	0.89360
H	6.84820	-3.53290	-1.13000

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Table S11 – *Continued from previous page*

Atom	Coordinates		
H	6.45160	-5.78720	-0.14870
C	0.13710	-0.57370	1.95020
H	0.70500	-1.48420	2.16650
H	0.44300	0.20900	2.65410
H	-0.92900	-0.77650	2.08990
C	0.33550	-0.52230	-2.00380
H	1.40400	-0.30310	-2.12070
H	0.04520	-1.26740	-2.75070
H	-0.23630	0.39540	-2.18730
C	0.69590	3.69350	0.24500
C	2.18140	3.92810	-0.20720
C	2.98870	2.70150	0.34510
F	3.49100	3.02390	1.57460
F	4.05520	2.41770	-0.44640
F	2.67890	5.10880	0.19900
F	2.22920	3.89410	-1.56100
F	-0.17330	4.25150	-0.63450
F	0.50170	4.33210	1.44020
H	-7.80520	0.19790	-0.58710
C	-6.94330	-2.10300	0.58030
O	-8.17830	-1.99080	0.41980
O	-6.27950	-3.02860	1.09750

Table S12: Atomic Cartesian coordinates for TS1 local maximum of *m*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.05016	-1.62889	-0.4361
C	-4.72414	-1.27672	-0.18187
C	-4.40395	-0.29601	0.76293
C	-5.42651	0.34252	1.47418
C	-6.7545	-0.00489	1.2263
C	-7.06149	-0.98299	0.27951
H	-3.94952	-1.79208	-0.75105
H	-5.17826	1.10777	2.21114
H	-7.55373	0.49439	1.77757
C	-2.98463	0.06088	0.99082
C	-2.22269	0.99363	0.35356
S	-2.0155	-0.80429	2.15545
C	-0.84717	0.99585	0.7679
H	-2.62281	1.63363	-0.42803
C	-0.5784	0.07514	1.75492
C	0.1819	1.84307	0.16019
C	1.37616	1.45947	-0.3426
C	1.90631	0.10217	-0.50538
C	3.2327	-0.25711	-0.09825
C	3.53007	-1.57558	-0.29477
H	3.9207	0.44304	0.36951
S	2.17177	-2.39097	-1.02144
C	1.20266	-0.9542	-1.03939
C	4.77797	-2.28534	0.02705
C	4.77838	-3.64334	0.37537
C	6.00245	-1.6015	-0.00519
C	5.96795	-4.29699	0.68675
H	3.83604	-4.19002	0.41966
C	7.18894	-2.25382	0.31692
H	6.02422	-0.55362	-0.30369
C	7.17821	-3.60528	0.66269
H	5.94682	-5.35291	0.95694
H	8.13067	-1.70538	0.28514

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Table S12 – *Continued from previous page*

Atom	Coordinates		
H	8.10861	-4.11706	0.90878
C	0.03736	3.34388	0.12127
C	1.20792	3.82766	-0.77373
C	2.21589	2.65232	-0.71068
F	1.73445	4.99908	-0.3726
F	0.77538	3.97395	-2.04605
F	2.88504	2.50624	-1.87935
F	3.16414	2.91619	0.24476
F	0.16121	3.87861	1.36959
F	-1.15426	3.76731	-0.36622
C	0.71446	-0.21635	2.45273
H	1.2286	-1.07603	1.99944
H	1.38747	0.64734	2.38991
H	0.5461	-0.44105	3.51287
C	-0.18156	-0.99742	-1.60505
H	-0.91179	-1.31877	-0.85007
H	-0.48111	-0.00329	-1.95531
H	-0.24274	-1.69322	-2.44959
C	-6.3838	-2.71441	-1.49288
O	-7.60176	-2.9613	-1.63505
O	-5.39246	-3.21088	-2.07489
H	-8.09013	-1.27425	0.06602

Table S13: Atomic Cartesian coordinates for TS2 local maximum of *m*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.21316	-1.21425	-0.07628
C	-4.85028	-1.11924	0.17714
C	-4.15779	0.09654	0.02156
C	-4.87014	1.23924	-0.40225
C	-6.23154	1.14892	-0.65435
C	-6.89816	-0.06975	-0.49275
H	-7.96677	-0.17224	-0.6841
H	-4.35666	-2.03871	0.49984
H	-4.36408	2.19447	-0.53219
H	-6.77858	2.03433	-0.98015
C	-6.95175	-2.56764	0.10447
O	-8.17437	-2.53364	-0.1482
O	-6.22417	-3.51175	0.47957
C	-2.73775	0.1866	0.2956
C	-1.90734	1.32393	0.14102
S	-1.81418	-1.16364	0.81989
C	-0.58614	1.09101	0.43834
H	-2.27366	2.27994	-0.22112
C	-0.27049	-0.27373	0.78078
C	0.53406	2.02108	0.1995
C	1.70751	1.56087	-0.34202
C	1.95653	0.20667	-0.68745
C	3.17828	-0.49146	-0.47871
C	3.09053	-1.85238	-0.43631
H	4.10868	0.03745	-0.28586
S	1.40667	-2.36209	-0.73798
C	0.79188	-0.68309	-0.81913
C	4.12783	-2.83587	-0.14818
C	3.82154	-4.19735	0.02833
C	5.48059	-2.45469	-0.03577
C	4.81568	-5.1306	0.31345
H	2.78791	-4.53455	-0.0535
C	6.46883	-3.38823	0.24898

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Table S13 – *Continued from previous page*

Atom	Coordinates		
H	5.76344	-1.41219	-0.17714
C	6.14698	-4.73635	0.42745
H	4.54231	-6.17793	0.4469
H	7.50618	-3.06077	0.3292
H	6.9251	-5.46689	0.64835
C	0.6489	-0.59382	1.94238
H	0.84688	-1.67191	1.98662
H	1.60472	-0.07474	1.8192
H	0.19786	-0.2763	2.89047
C	-0.15755	-0.46519	-1.98601
H	0.36222	-0.76385	-2.90271
H	-1.07312	-1.06215	-1.89974
H	-0.42399	0.59201	-2.08168
C	0.52202	3.47478	0.42448
C	2.01581	3.88256	0.29216
C	2.66714	2.71142	-0.50073
F	3.91874	2.45159	-0.03421
F	2.80651	3.06238	-1.80817
F	2.57266	3.95879	1.52428
F	2.1924	5.07396	-0.31116
F	-0.23127	4.17898	-0.49833
F	0.01295	3.84417	1.63669

Table S14: Atomic Cartesian coordinates for TS3 local maximum of *m*-DTE$^-$ calculated at the ωB97X-D/aug-cc-pVDZ level of theory.

Atom	Coordinates		
C	-6.37579	-0.75899	0.13373
C	-5.02537	-1.02109	0.35594
C	-4.02816	-0.11989	-0.05451
C	-4.41065	1.06421	-0.7162
C	-5.75469	1.31567	-0.96707
C	-6.73016	0.41251	-0.53886
H	-4.7719	-1.93792	0.88768
H	-3.65941	1.76691	-1.07773
H	-6.04163	2.22204	-1.50292
C	-2.602	-0.41847	0.19251
C	-1.7462	0.71924	0.44574
S	-2.04414	-1.99747	0.07135
C	-0.37975	0.77351	0.47867
H	-2.25444	1.68118	0.51055
C	0.62862	-0.37165	0.44741
C	0.40917	1.96735	0.4375
C	1.74187	1.67645	0.24527
C	1.97677	0.29055	0.19503
C	3.16008	-0.47699	0.17755
C	3.14468	-1.79719	-0.18942
H	4.09742	-0.02148	0.49718
S	1.74895	-2.37429	-1.09373
C	0.60559	-1.10363	-0.85322
C	4.25054	-2.75628	-0.01262
C	4.00102	-4.11093	0.25017
C	5.58549	-2.33041	-0.10946
C	5.05251	-5.01055	0.41529
H	2.97289	-4.45998	0.34671
C	6.6325	-3.22902	0.06369
H	5.80492	-1.28902	-0.34354
C	6.37266	-4.5752	0.32641
H	4.83439	-6.05813	0.62348
H	7.66125	-2.87756	-0.01929

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Table S14 – *Continued from previous page*

Atom	Coordinates		
H	7.19471	-5.27863	0.4581
C	0.63317	-1.15213	1.76846
H	-0.35893	-1.54465	1.99238
H	1.34617	-1.98269	1.73182
H	0.94984	-0.46348	2.56233
C	-0.05682	-0.59234	-2.09843
H	0.55651	0.21143	-2.53454
H	-0.12288	-1.3938	-2.84386
H	-1.05586	-0.19618	-1.90178
C	0.14127	3.42827	0.38532
C	1.57549	4.04865	0.52784
C	2.55874	2.91452	0.07742
F	3.70195	2.92917	0.81047
F	2.9235	3.11273	-1.22035
F	1.80456	4.33714	1.82912
F	1.73051	5.17843	-0.18394
F	-0.40516	3.82514	-0.80417
F	-0.68542	3.88692	1.35773
H	-7.7927	0.58675	-0.71048
C	-7.46803	-1.74719	0.62509
O	-8.63862	-1.43391	0.31316
O	-7.04285	-2.72887	1.2712

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