Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

E/Z photoisomerization pathway in pristine and fluorinated di(3-furyl)ethenes

S. M. Sudarkova, I. N. Ioffe

Supporting information contains the Cartesian coordinates of the key points in the S1 state of the pristine and fluorinated di(3-furyl)ethenes (3DFE), obtained at the XMCQDPT2 level of theory, as well as schematic representations of S1 surface of 2F-3DFE and 8F-3DFE along the E/Z photoisomerization path (XMCQDPT2 data).

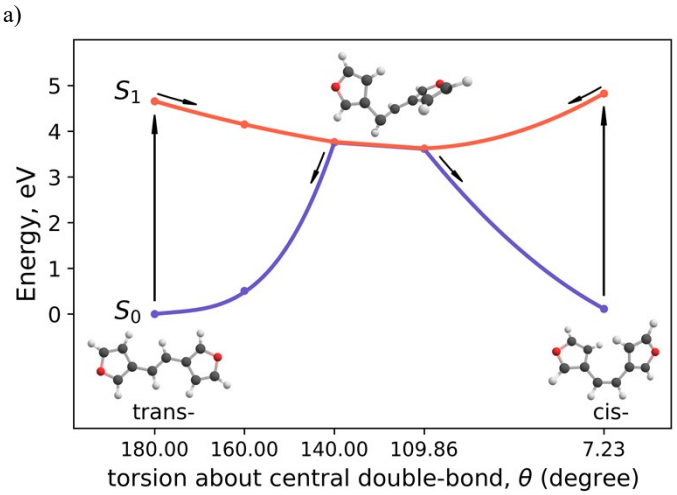

Fig. 3. a) Key points of the S0 and S1 potential energy surfaces in 3DFE along the E/Z isomerization pathway in S1, obtained at the XMCQDPT2 level of theory.

Table S1. Cartesian coordinates of the key points in the S_1 state of 3DFE, see Fig. 3a of the main text.

180.00 degrees of torsion angle				160.00 degrees of torsion angle			
C	0.522498927	-1.287441166	-2.038567570	C	0.433164731	-1.482732508	-2.040955883
C	-0.250389949	-0.267945085	-2.692603031	C	-0.584271862	-0.699432148	-2.718575399
C	0.173564733	-0.231247260	-3.973163652	C	-0.264358848	-0.699028249	-4.042872593
O	1.150413303	-1.143223416	-4.181933272	O	0.892778552	-1.416895968	-4.273336974
C	1.350601285	-1.773292768	-3.006025168	C	1.307054154	-1.885513998	-3.075325602
H	-1.018845093	0.352587955	-2.261749152	H	-1.442195432	-0.228451764	-2.267773476
H	-0.107452568	0.363079745	-4.826008152	H	-0.712242085	-0.267913202	-4.920130142
C	0.377737892	-2.719030101	2.305004188	C	-0.019348790	-3.007934576	2.066974375
C	-0.395151438	-1.699534420	1.650968534	C	-0.575291147	-1.768212995	1.557877365
C	-1.223260417	-1.213689384	2.618423733	C	-1.349999790	-1.269870938	2.627710239
O	-1.023075745	-1.843761969	3.794330680	O	-1.297060508	-2.098053239	3.695055947
C	-0.046222633	-2.755733648	3.585562693	C	-0.485873236	-3.157287282	3.337860399
H	1.146200054	-3.339556171	1.874152800	H	0.619827547	-3.694254085	1.535993929
H	0.234792790	-3.350062476	4.438406543	H	-0.357553827	-3.906454602	4.098490833
C	0.472190779	-1.735450286	-0.666060844	C	0.529426683	-1.772744201	-0.670141617
C	-0.344841817	-1.251523882	0.278462325	C	-0.385125416	-1.194267212	0.289911198
H	1.164546309	-2.531058658	-0.405895030	H	1.339943644	-2.402745453	-0.314183461
H	-1.037197174	-0.455915337	0.018296612	H	-0.894916797	-0.266972037	0.042559983
H	-1.979286145	-0.446368136	2.611088671	H	-1.936336100	-0.372780850	2.747672822
H	2.106626101	-2.540614918	-2.998690493	H	2.219549641	-2.460053783	-3.075076384
140.00 degrees of torsion angle				109.86 degrees of torsion angle			
C	0.352520724	-1.748985635	-2.083992179	C	0.252413447	-2.300107045	-1.865084617
C	-0.935944894	-1.733020742	-2.737203748	C	-1.103031983	-2.722987841	-2.195641562
C	-0.701675905	-1.454061048	-4.059066263	C	-1.239371820	-2.593258478	-3.547254622

O	0.630161897	-1.301804085	-4.295310998	O	-0.087444151	-2.122118615	-4.108342538
C	1.260155395	-1.474101676	-3.085646426	C	0.792360512	-1.909462067	-3.082806713
H	-1.896038216	-1.919694025	-2.281895369	H	-1.844597011	-3.115359496	-1.517924857
H	-1.339560261	-1.338738598	-4.916663119	H	-2.042538468	-2.790458819	-4.234514278
C	-0.744721094	-3.334492919	1.817801448	C	-1.008233193	-3.471085205	1.605105784
C	-0.607298349	-1.929473782	1.506125608	C	-1.002147715	-2.122450828	1.070600342
C	-1.146212169	-1.248750208	2.586077433	C	-2.083814617	-1.486715711	1.661785652
O	-1.598416577	-2.100675118	3.511615702	O	-2.719882056	-2.308105373	2.497469156
C	-1.344444648	-3.388861947	3.029156300	C	-2.051124964	-3.528586889	2.455104425
H	-0.407774053	-4.141607626	1.191067003	H	-0.298733268	-4.236331855	1.342942057
H	-1.657934754	-4.179944870	3.684729150	H	-2.471851169	-4.287903588	3.088216053
C	0.624097817	-2.090119576	-0.669675751	C	0.926516787	-2.384398196	-0.525829291
C	-0.058270556	-1.338192600	0.346269492	C	-0.097737323	-1.573008447	0.139657235
H	1.534331094	-1.432186911	-0.439490615	H	1.851454085	-1.792999223	-0.597976496
H	-0.076557098	-0.233069602	0.359305324	H	-0.305603112	-0.528579110	-0.145269386
H	-1.250814563	-0.198313454	2.802537162	H	-2.482115391	-0.490121546	1.567102460
H	2.333935802	-1.406758893	-3.104784546	H	1.774476249	-1.575961110	-3.368878311

7.23 degrees of torsion angle

C	0.080909525	-2.731504017	-1.794581075
C	-1.166887763	-3.204856853	-2.328433350
C	-0.856605851	-4.037117573	-3.345070565
O	0.484781343	-4.127946375	-3.497219611
C	1.035675320	-3.328160487	-2.563781610
H	-2.157517073	-2.932858165	-2.006266197
H	-1.450425787	-4.611221296	-4.035854425
C	-2.209007504	-3.243040827	0.683728607
C	-1.645289106	-1.925879378	0.799974868
C	-2.516239734	-1.245266327	1.598402030
O	-3.557942245	-2.019038107	1.959776259
C	-3.353060411	-3.233808893	1.400287785
H	-1.793554822	-4.084260605	0.155637791
H	-4.097878862	-3.982480523	1.610399961
C	0.354416656	-1.762986363	-0.747923005
C	-0.392498942	-1.387301426	0.301045563
H	1.305319496	-1.250139027	-0.858505033
H	0.004693164	-0.569615575	0.895228579
H	-2.519488808	-0.235352371	1.973668434
H	2.111821426	-3.277057431	-2.554403188

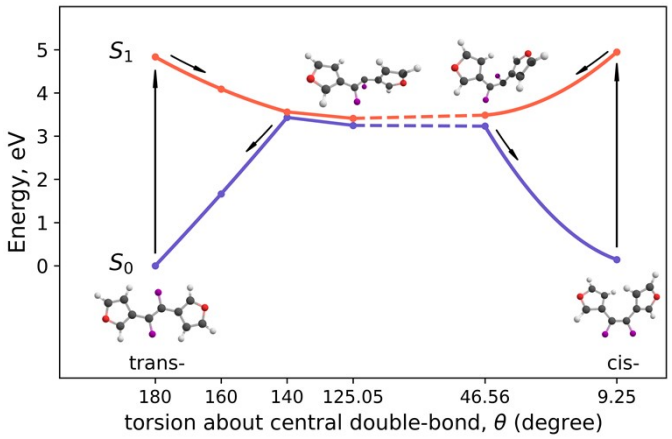

Fig. S1. Schematic representation of S_1 surface of 2F-3DFE along the E/Z photoisomerization path (XMCQDPT2 data). Vertical excitation is followed by, relaxation in the S_1 state, which leads to the two different S_0/S_1 intersection domains, depending on the stating isomer, E or Z.

Table S2. Cartesian coordinates of the key points in the S_1 state of 2F-3DFE, see Fig. S1.

180.00 degrees of torsion angle				160.00 degrees of torsion angle			
C	0.515769451	-1.269303241	-2.069771200	C	0.362427850	-1.551530128	-2.098948103
C	-0.247084397	-0.254654617	-2.740122053	C	-0.773414318	-1.047790673	-2.835715492
C	0.196809021	-0.239999951	-4.014588872	C	-0.364689004	-0.937282258	-4.127212036
O	1.171954692	-1.159447121	-4.195901492	O	0.952642088	-1.336960544	-4.262355968
C	1.358009883	-1.776759112	-3.015305602	C	1.372895506	-1.713940615	-3.037599210
C	0.393970678	-2.745089201	2.333697152	C	-0.360486061	-3.212123173	1.971517883
C	-0.368888398	-1.730445360	1.663344923	C	-0.634417563	-1.860134504	1.542990963
C	-1.211136126	-1.222997200	2.608876933	C	-1.152124265	-1.214061260	2.657608683
O	-1.025080756	-1.840309633	3.789472590	O	-1.195900788	-2.048713863	3.717111951
C	-0.049927446	-2.759749145	3.608162254	C	-0.714857290	-3.270120439	3.282836142
C	0.464748736	-1.714915029	-0.703210500	C	0.442434523	-1.834913423	-0.713407041
C	-0.317866409	-1.284832206	0.296784746	C	-0.433748077	-1.299000210	0.257407968
H	-1.015595470	0.369036982	-2.319386290	H	-1.738368249	-0.795388790	-2.428880946
H	-0.069890461	0.343766404	-4.878903312	H	-0.836151295	-0.607791279	-5.035280327
H	2.108298097	-2.546924866	-2.982909404	H	2.392061913	-2.050940164	-2.955715261
H	-1.961429575	-0.452836603	2.576479303	H	-1.487998767	-0.204269836	2.820215698
H	1.162488584	-3.368773839	1.912963548	H	0.058241669	-4.001568836	1.369934855
H	0.216772806	-3.343515265	4.472476620	H	-0.692821347	-4.043069083	4.029593287
F	1.336626135	-2.702197403	-0.420758999	F	1.756825292	-2.153720220	-0.315035494
F	-1.189744683	-0.297550658	0.014332905	F	-0.651371504	0.094857149	0.248354762
140.00 degrees of torsion angle				125.05 degrees of torsion angle			
C	0.390368125	-1.785273593	-2.031198120	C	0.168604714	-2.251215801	-2.010140954
C	-0.867560924	-1.944511173	-2.720406825	C	-1.072396180	-2.663205467	-2.621810705
C	-0.680718899	-1.458003633	-3.983151035	C	-0.977689181	-2.342417378	-3.947657062
O	0.593471458	-1.022216752	-4.155436695	O	0.230942181	-1.781064697	-4.229147438
C	1.233855587	-1.211643754	-2.949430434	C	0.912155322	-1.703595209	-3.037191894
C	-0.662847376	-3.334406946	1.874589448	C	-1.104263517	-3.454765314	1.790804906
C	-0.596777977	-1.947077798	1.485972619	C	-1.067731501	-2.106446253	1.276462464
C	-1.230677245	-1.226002039	2.497940258	C	-1.960712333	-1.373062786	2.055341767
O	-1.663587252	-2.042815277	3.442645076	O	-2.518586180	-2.146972621	2.971723118
C	-1.312667543	-3.350078557	3.065148941	C	-1.987781039	-3.434670125	2.814019071
C	0.703718382	-2.261565659	-0.675269435	C	0.577344973	-2.494956628	-0.617584455
C	0.005268661	-1.425348825	0.326270414	C	-0.279086016	-1.628840304	0.220064681
H	-1.773826476	-2.384839285	-2.335104262	H	-1.902917873	-3.157694722	-2.143023682
H	-1.325965132	-1.373126979	-4.839900827	H	-1.644043193	-2.461718974	-4.783487541
H	2.274095101	-0.944443412	-2.920965546	H	1.916119052	-1.324730269	-3.090286951
H	-1.420959684	-0.174141033	2.631975850	H	-2.266292898	-0.340310984	2.032454222
H	-0.259080949	-4.150399351	1.302077127	H	-0.528992083	-4.275139087	1.399871958
H	-1.611659979	-4.108011790	3.764434066	H	-2.366648967	-4.159127007	3.510171535
F	2.050406805	-1.804284517	-0.308397724	F	1.896817524	-1.974932307	-0.392863323
F	-0.046629865	-0.112401840	0.256853179	F	-0.435741568	-0.331917450	-0.002640081
46.56 degrees of torsion angle				9.25 degrees of torsion angle			
C	0.207719946	-2.631827276	-1.510469807	C	0.204617890	-2.756121368	-1.702307993
C	-1.139067625	-2.676376073	-2.039395576	C	-1.030439316	-3.188056541	-2.291454605
C	-1.062038183	-3.396467486	-3.171570596	C	-0.696871184	-4.090150259	-3.238595301
O	0.255949364	-3.819707514	-3.398427153	O	0.644734094	-4.251190749	-3.295282640
C	0.987494091	-3.353661684	-2.402149005	C	1.179833833	-3.438493300	-2.366515376
C	-1.560114147	-3.079079422	1.487552297	C	-2.167327249	-3.114517506	0.692713823
C	-1.404798230	-1.775273935	0.886218672	C	-1.623763663	-1.787174952	0.734972567
C	-2.692971421	-1.275117104	0.760672945	C	-2.542734828	-1.041867278	1.411618967
O	-3.615234528	-2.171818862	1.269569743	O	-3.596489776	-1.796390688	1.771507150
C	-2.909031899	-3.258295415	1.686240248	C	-3.356393937	-3.051432945	1.328456075
C	0.648715639	-1.972315940	-0.357350692	C	0.453017943	-1.747928384	-0.697323277
C	-0.143191184	-1.118097831	0.562972143	C	-0.345290229	-1.292088055	0.278003644
H	-2.004501241	-2.222916215	-1.586623617	H	-2.023454253	-2.851470809	-2.047401265
H	-1.763971499	-3.716759785	-3.918617997	H	-1.274161149	-4.672572251	-3.936042704
H	2.040037346	-3.584027782	-2.418797906	H	2.253281786	-3.427695901	-2.292265661
H	-3.083212261	-0.322799664	0.451575008	H	-2.562886656	-0.007794052	1.708768711
H	-0.778228350	-3.765361156	1.774023149	H	-1.715755234	-3.991427117	0.261376054
H	-3.486813028	-4.061073073	2.109123791	H	-4.112531993	-3.785058347	1.549727803
F	1.927701078	-2.109714077	-0.126141092	F	1.670605967	-1.186186291	-0.797363280
F	-0.384060177	-0.019276203	-0.359765259	F	0.090950214	-0.225700641	0.971262067

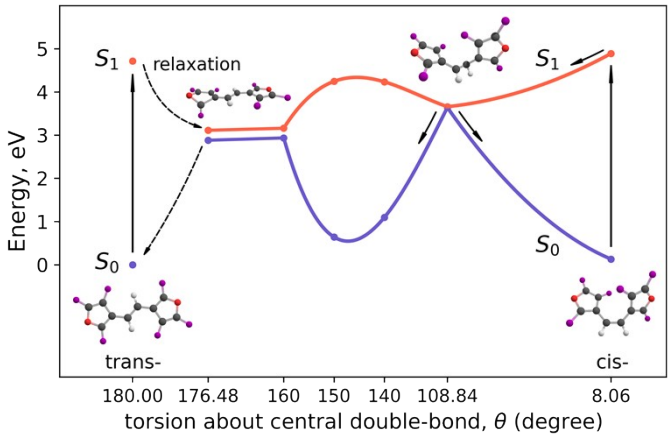

Fig. 4. Key points of the S_0 and S_1 surfaces in 6F-3DFE along the E/Z isomerization pathway in S_1, obtained at the XMCQDPT2 level of theory.

Table S3. Cartesian coordinates of the key points in the S_1 state of 6F-3DFE, see Fig. 4 of the main text.

180.00 degrees of torsion angle				176.48 degrees of torsion angle			
C	0.515071168	-1.278157567	-2.044046975	C	0.542819664	-1.380369876	-1.957221861
C	-0.248201107	-0.257771949	-2.727236278	C	-0.072531219	-0.341291439	-2.661196802
C	0.173436879	-0.220655039	-4.001737360	C	0.068807306	-0.603387596	-4.024422319
O	1.150094369	-1.133401982	-4.207309815	O	0.712708950	-1.736158436	-4.316333419
C	1.326736170	-1.741344748	-3.027061388	C	1.477502465	-1.942850314	-3.054063968
C	0.375368915	-2.721782375	2.319643973	C	0.250151528	-2.826153585	2.349743945
C	-0.387961395	-1.701458506	1.636439437	C	-0.388666430	-1.704598601	1.688857601
C	-1.199596151	-1.238234343	2.619462815	C	-1.156648010	-1.170810036	2.696472628
O	-1.022899447	-1.846131474	3.799728955	O	-1.061506241	-1.827828181	3.872579929
C	-0.046221985	-2.758857205	3.594164163	C	-0.185660058	-2.847505442	3.633931891
C	0.472440317	-1.732009549	-0.677230313	C	0.488572352	-1.825707247	-0.632258187
C	-0.345301829	-1.247559348	0.269632111	C	-0.284393573	-1.221948445	0.345391086
H	1.168214884	-2.526161962	-0.432744931	H	1.088489644	-2.692964909	-0.389354969
H	-1.041082643	-0.453406850	0.025172372	H	-0.859502122	-0.337261289	0.103086676
F	-1.190399895	0.498688826	-2.187135218	F	-0.749413700	0.709755537	-2.197951633
F	-0.161373421	0.494834622	-5.037972515	F	-0.224996193	0.205528391	-5.007647824
F	2.242910249	-2.669855898	-3.021445664	F	2.555120968	-1.118916205	-3.132489221
F	1.317554809	-3.478261409	1.779544585	F	1.109984071	-3.675492168	1.795467562
F	0.288652411	-3.474299778	4.630417337	F	0.066271850	-3.627015149	4.654526118
F	-2.115785222	-0.309732859	2.613843405	F	-1.965860025	-0.139594562	2.703736991
160.00 degrees of torsion angle				150.00 degrees of torsion angle			
C	0.388266908	-1.587592326	-2.020623844	C	0.349566111	-1.596967294	-2.083364346
C	-0.322426146	-0.622729630	-2.746586276	C	-0.678650314	-0.904837061	-2.831680613
C	-0.291923265	-0.988959933	-4.090125626	C	-0.310719843	-0.890934677	-4.141263769
O	0.368350193	-2.119431328	-4.352419935	O	0.874861549	-1.558079976	-4.338162224
C	1.246496862	-2.208386749	-3.151807874	C	1.213720398	-2.014879437	-3.114779371
C	-0.024264461	-3.082955747	2.222662167	C	-0.203525037	-3.125383656	2.046530945
C	-0.528274754	-1.871027908	1.605959396	C	-0.661265857	-1.864977098	1.500463260
C	-1.347929713	-1.363259450	2.587322357	C	-1.450787962	-1.371364332	2.558127232
O	-1.411824347	-2.122606338	3.702551932	O	-1.412635549	-2.127273750	3.674980385
C	-0.582766335	-3.178753448	3.454888075	C	-0.651029297	-3.217703426	3.327865323
C	0.469803847	-1.924298540	-0.670498735	C	0.510098662	-1.801582861	-0.700318635
C	-0.279313927	-1.299361519	0.319157312	C	-0.397859430	-1.238321233	0.268301130
H	1.070238325	-2.791922839	-0.427388182	H	1.344692271	-2.412400611	-0.371721339
H	-0.829096938	-0.397856450	0.078793552	H	-0.909892366	-0.305720065	0.054493502
F	-0.985622625	0.446147856	-2.305060356	F	-1.780747353	-0.351047369	-2.333251439
F	-0.716651142	-0.280321312	-5.102204601	F	-0.898484575	-0.467044290	-5.229579132
F	2.284809670	-1.365699631	-3.386919433	F	2.431538619	-2.487656836	-3.020812095
F	0.830850126	-3.941737128	1.675903607	F	0.547406496	-4.029782457	1.423791609
F	-0.475638060	-4.052384911	4.423330716	F	-0.584225080	-4.160353516	4.231458412
F	-2.098111304	-0.288573873	2.606761454	F	-1.933396325	-0.165311199	2.725409047

140.00 degrees of torsion angle			
C	0.322861546	-1.670026415	-2.079233593
C	-0.814350659	-1.153416193	-2.817812372
C	-0.500469518	-1.182230640	-4.139032840
O	0.753059218	-1.708791643	-4.345216727
C	1.195197144	-2.031650232	-3.113172270
C	-0.424665262	-3.228244349	1.911246888
C	-0.716072235	-1.877631752	1.467597235
C	-1.451135401	-1.375602692	2.546313249
O	-1.558439378	-2.225498643	3.586093300
C	-0.925531640	-3.371731236	3.165690508
C	0.540778434	-1.785772980	-0.691574441
C	-0.366431526	-1.206747941	0.277473306
H	1.471111524	-2.249354281	-0.363134860
H	-0.729458064	-0.187579699	0.145398124
F	-1.956454426	-0.715543556	-2.297265068
F	-1.168164530	-0.894027855	-5.226907754
F	2.454745687	-2.385079070	-3.053337344
F	0.230976353	-4.156707637	1.221841838
F	-0.987084111	-4.378743427	3.999117032
F	-1.859657530	-0.154993664	2.783771938

108.84 degrees of torsion angle			
C	-0.163982501	-1.856644082	-1.931244853
C	-1.303896322	-1.973250609	-2.838987067
C	-0.895792333	-2.736157020	-3.877615387
O	0.432020695	-3.138404155	-3.715041009
C	0.820753284	-2.608303641	-2.572751284
C	-1.571257034	-3.203806718	0.919049794
C	-1.264082878	-1.802945974	1.120439019
C	-1.337112106	-1.700956775	2.505636403
O	-1.833427541	-2.826709175	3.112794347
C	-1.956608407	-3.738256469	2.109996535
C	-0.031787918	-1.303022893	-0.655260204
C	-1.159601507	-0.734117741	0.096893036
H	0.965140587	-1.452838410	-0.210958910
H	-0.800632002	0.177290734	0.597390563
F	-2.491085978	-1.438704491	-2.702263941
F	-1.452177535	-3.168033245	-4.970149399
F	2.030985915	-2.880952193	-2.211363293
F	-1.558837035	-3.841541236	-0.265143279
F	-2.152590231	-4.984687607	2.493730511
F	-1.475448204	-0.604897303	3.235290854

8.06 degrees of torsion angle			
C	0.002731150	-2.610355268	-1.882120949
C	-1.262519834	-3.016550546	-2.451390990
C	-0.997992236	-3.791272907	-3.515854691
O	0.337582659	-3.920962199	-3.690125442
C	0.897100656	-3.200310094	-2.712531771
C	-2.071191820	-3.378737516	0.802407493
C	-1.558785791	-2.028642921	0.870089586
C	-2.440110891	-1.425555721	1.705031309
O	-3.421946130	-2.227603966	2.130221215
C	-3.174379299	-3.432409997	1.566177933
C	0.324360474	-1.712822017	-0.791491770
C	-0.360316384	-1.424808182	0.324506351
H	1.257883642	-1.176550433	-0.926818057
H	0.050781990	-0.632992187	0.942077473
F	-2.458065149	-2.653056244	-2.023073345
F	-1.746171698	-4.408107392	-4.386898500
F	2.201662132	-3.189920581	-2.716546413
F	-1.524779630	-4.383471530	0.141466789
F	-4.013359470	-4.383152025	1.868168352
F	-2.496560834	-0.202784300	2.156316033

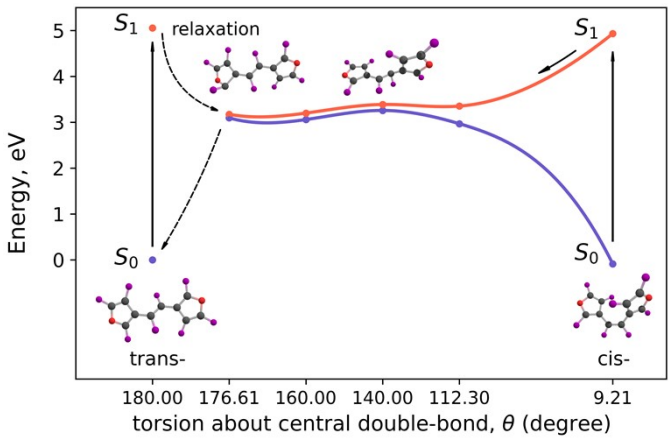

Fig. S2. Schematic representation of S_1 surface of 8F-3DFE along the E/Z photoisomerization path (XMCQDPT2 data).

Table S4. Cartesian coordinates of the key points in the S_1 state of 8F-3DFE, see Fig. S2.

180.00 degrees of torsion angle				176.61 degrees of torsion angle			
C	0.441246079	-1.290628497	-2.088949487	C	0.480977972	-1.334344051	-2.015920647
C	-0.352007251	-0.320363303	-2.810808696	C	-0.066618395	-0.275467301	-2.740207080
C	0.183307175	-0.209809034	-4.038071155	C	0.723271129	-0.102583762	-3.884700316
O	1.251181816	-1.030562604	-4.169612886	O	1.771512579	-0.918970366	-3.981147951
C	1.377519871	-1.659393239	-2.998699242	C	1.303531893	-2.044417541	-3.120787807
C	0.491831692	-2.668362226	2.393522944	C	0.650179338	-2.422134569	2.506378840
C	-0.301419890	-1.698094830	1.671664877	C	-0.357403670	-1.751880241	1.707746305
C	-1.237697183	-1.329334440	2.581412783	C	-1.400438038	-1.600765362	2.587524561
O	-1.111362087	-1.958168879	3.752324700	O	-1.149351798	-2.105870909	3.812467632
C	-0.043486381	-2.778921148	3.620783398	C	0.118125979	-2.606339405	3.741908959
C	0.286424300	-1.818560457	-0.751671479	C	0.396688401	-1.815773715	-0.701954708
C	-0.146598308	-1.170162926	0.334386827	C	-0.329547267	-1.289620209	0.344745469
F	0.627374373	-3.107350932	-0.623329666	F	1.106761350	-2.921212924	-0.430845505
F	-0.487548124	0.118627620	0.206045088	F	-1.113404221	-0.235624233	0.080449620
F	-0.123578860	0.494105391	-5.089592349	F	0.433216583	0.655079731	-4.907264550
F	-1.423390807	0.300428195	-2.363568306	F	-1.123826304	0.490357833	-2.510826062
F	2.363815966	-2.502760455	-2.933402881	F	0.433477768	-2.759316965	-3.875664295
F	1.563218194	-3.289149868	1.946284244	F	1.880945845	-2.732321697	2.131564123
F	0.263398130	-3.482837559	4.672303707	F	0.586161513	-3.122292802	4.849410246
F	-2.223994368	-0.485968551	2.516115927	F	-2.590709252	-1.080307485	2.440264121
160.00 degrees of torsion angle				140.00 degrees of torsion angle			
C	0.408935129	-1.274762353	-2.002780676	C	0.223338804	-1.598401258	-2.005836708
C	-0.580994011	-0.780591587	-2.852875340	C	-0.946607155	-1.419218909	-2.861786453
C	0.044559206	-0.419297688	-4.051814627	C	-0.540836535	-1.694335982	-4.121131327
O	1.365039200	-0.578173290	-4.073127286	O	0.814237117	-2.043965007	-4.144934518
C	1.527487941	-1.622948401	-3.009782413	C	1.225696345	-1.977587198	-2.901631758
C	-0.101041977	-2.960242416	2.207108072	C	-0.815345598	-3.137614372	1.597106263
C	-0.547879277	-1.692384623	1.664572616	C	-0.746497501	-1.704245633	1.508094589
C	-1.186456436	-1.106351561	2.730848828	C	-0.915658577	-1.318439912	2.813173643
O	-1.180485124	-1.865879183	3.845457172	O	-1.172971199	-2.370627328	3.663665733
C	-0.506662608	-3.002167629	3.502512934	C	-1.107325507	-3.477023289	2.882320832
C	0.503335153	-1.492225160	-0.625011893	C	0.369889770	-1.451760807	-0.625468470
C	-0.426179667	-1.151350838	0.341228082	C	-0.718257700	-0.951219633	0.252268634
F	1.584723584	-2.159544228	-0.194462002	F	-2.151208869	-1.061373756	-2.510240179
F	-1.391610397	-0.294935382	-0.025104239	F	-1.113069302	-1.706191360	-5.284776773
F	-0.556593602	-0.094437940	-5.163649348	F	2.460270918	-2.267720693	-2.700610388
F	-1.887924427	-0.651315567	-2.673916411	F	-0.604707425	-3.960605947	0.551090224
F	1.192618490	-2.799189400	-3.595147977	F	-1.105163834	-4.634415125	3.516179466
F	0.516165180	-3.927106217	1.547229315	F	-1.187230337	-0.136613027	3.340228741
F	-0.407035900	-3.906784807	4.442196961	F	1.590172023	-1.685764795	-0.196573541
F	-1.782818852	0.050183606	2.855401145	F	-0.155092761	0.370955089	0.462473262
112.30 degrees of torsion angle				9.31 degrees of torsion angle			
C	-0.095173457	-1.901932373	-1.972679296	C	1.650629298	-2.233406465	-0.952514241
C	-1.233266972	-1.931554996	-2.886620149	C	2.916894132	-2.192946948	-0.257967196
C	-0.845990682	-2.660476451	-3.956241842	C	3.879539304	-2.376433302	-1.176466177
O	0.463505472	-3.123399531	-3.799945540	O	3.336743965	-2.540769847	-2.404829849
C	0.874861954	-2.654443864	-2.643216787	C	2.014472533	-2.450611714	-2.239827594
C	-1.674498905	-3.269954941	1.037928257	C	1.403609424	0.797373333	0.466016526
C	-1.281919554	-1.888523164	1.179007040	C	0.587223370	-0.203457832	1.113474474
C	-1.295081677	-1.720232849	2.557423801	C	0.583545469	0.195623496	2.408624913
O	-1.795631537	-2.810388186	3.225758044	O	1.297283536	1.304590345	2.619577880
C	-1.991097020	-3.753993033	2.267610024	C	1.799418142	1.661605150	1.414986339
C	0.009945289	-1.383264649	-0.681311691	C	0.308374685	-2.148659725	-0.419149134
C	-1.161523345	-0.931220471	0.080455541	C	-0.128460261	-1.319363536	0.533952179
F	-2.391547298	-1.344501125	-2.740159140	F	-0.556051687	-3.025349708	-0.941761752
F	-1.403391930	-3.007823457	-5.075812182	F	-1.366075468	-1.496007288	1.009545539
F	2.057251243	-3.008829500	-2.282767158	F	5.178431134	-2.438128288	-1.116487176
F	-1.707752383	-3.941033165	-0.125703710	F	3.079766155	-2.031314578	1.041338608
F	-2.250109977	-4.970195501	2.702989014	F	1.314654271	-2.589913914	-3.324921799
F	-1.325831928	-0.615202816	3.276833563	F	1.678539400	0.853612800	-0.823200449
F	1.227797833	-1.524235237	-0.161458576	F	2.530270482	2.738686319	1.400827190
F	-0.952003757	0.389615653	0.518553587	F	0.012743925	-0.299565664	3.464806798