

## Electronic Supplementary Information

# Parallel Ultrafast *E-C* Ring Closure and *E-Z* Isomerisation in a Photochromic Furylfulgide Studied by Femtosecond Time-Resolved Spectroscopy

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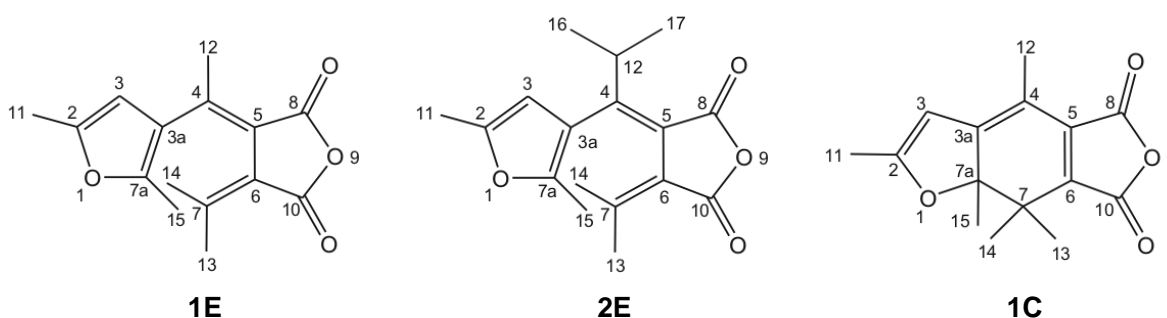
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## 1. $^1\text{H}$ and $^{13}\text{C}$ NMR data

The molecule of interest 1-[1-(2,5-dimethyl-3-furyl)-ethylidene]-2-isopropylidene succinic anhydride (**1E**) has been obtained quantitatively by irradiating the closed 7,7a-dihydro-2,4,7,7,7a-pentamethylbenzo[b]furan-5,6-dicarboxylic anhydride (**1C**) at  $\lambda = 500$  nm in  $\text{CDCl}_3$ . NMR data were acquired on Bruker Avance 600 MHz and DRX-500 spectrometers. For comparison, samples of 1-[1-(2,5-dimethyl-3-furyl)-2-methylpropylidene]-2-isopropylidene succinic anhydride (**2E**) were measured under the same conditions. The numbering of **1E** and **2E** has been taken from **1C** and is given in Figure S1.



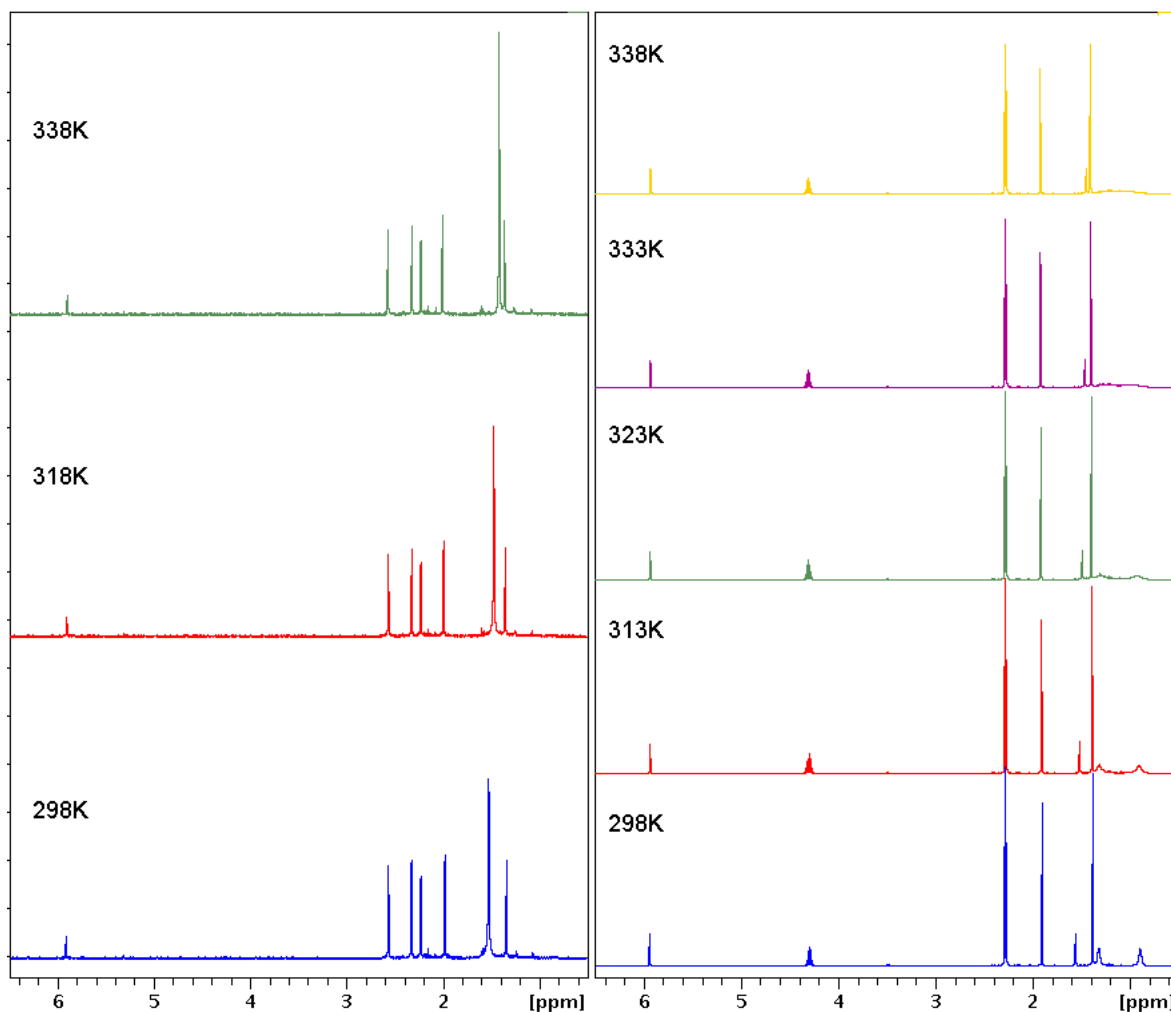
**Figure S1.** Structures and numbering of **1E**, **2E** and **1C**.

The assignment of the  $^1\text{H}$  and  $^{13}\text{C}$ -chemical shifts were made by analysis of  $^1\text{H}$ -1D-NMR, natural abundance  $^1\text{H}$ ,  $^{13}\text{C}$ -HSQC and  $^1\text{H}$ ,  $^{13}\text{C}$ -HMBC experiments. The assignments are complete and unambiguous, and are based largely on  $^3\text{-}^5\text{J}$ -correlations in the HMBC experiment with the exception of the isopropyliden-methyl groups, which were distinguished based on the NOE intensities in a 2D-NOESY experiment owing to the conformation-independent closer proximity of 14-H to all other protons in the compound.

The assignments are collected in Table S1. Figure S2 shows the 1D  $^1\text{H}$  NMR data measured at temperatures from 298 to 338 K.

**Table S1.** Chemical Shifts of **1E**.

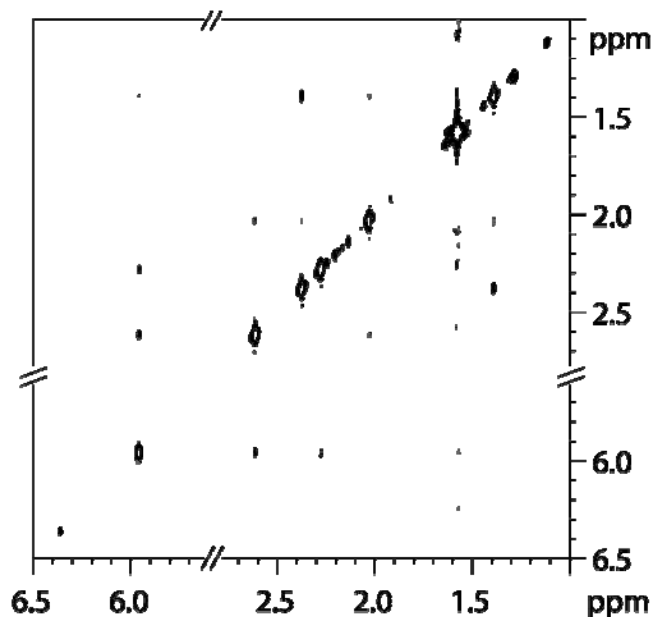
Atom number	<sup>13</sup> C-Verschiebung (ppm)	<sup>1</sup> H-Verschiebung (ppm)
7a	148.14	
3a	124.01	
3	105.7	5.927
2	151.05	
4	146.62	
5	119.12	
6	120.84	
7	153.49	
8	163.70	
10	163.14	
15	13.82	2.000
11	13.22	2.247
12	22.08	2.582
14	26.71	1.358
13	22.54	2.344



**Figure S2.** 500 MHz  $1D$ - $^1H$ -NMR Spectra for **1E** (left) and **2E** (right) at temperatures from 298 to 338 K.

As seen in Fig. S2, a single set of uniformly sharp resonances persists at temperatures up to 338 K. This suggests a fast interconversion between the two **1E** conformers. Published results show that the thermal enantiotopomerisation of the chemically very similar furylfulgide 1-[1-(2,5-dimethyl-3-furyl)-2-methylpropylidene]-2-isopropylidene succinic anhydride (**2E**) occurs with a barrier of 52.9 kJ/mol [1, 2]. Since the isopropyl-group in **2E** is not expected to have a significant effect on either the furyl-group rotation or the inversion of the helical chirality, a similarly fast process is very likely for **1E**, which is consistent with our NMR data. The 2D-NOESY data are shown in Fig. S3, the NOE cross peak intensities derived from the data are given in Table S2.

In the isopropyl-furylfugid, the presence of a prochiral-group allows to directly assess the chirality of the molecule. Notably, as previously published, the prochiral methyl groups of the isopropyl groups are chemically inequivalent at room temperature confirming the chirality. They are broadened due to slow interconversion, which is substantiated by exchange cross peaks in a 2D-NOESY spectrum (data not shown). The resonance broadening increases with elevating temperature, and the estimated coalescence temperature was  $\sim 65$  C/500 MHz, which is consistent with the published rotational barrier for the furyl group of 52.9 kJ/mol [1, 2]. This conformational barrier is too high to originate in hindered rotation of the isopropyl group itself, which is also confirmed by the observation that the methine-proton of this group is not broadened at any temperature. Thus, the underlying isomerization is remote, and can be assigned to the furyl-ring rotation / diastereotopomerization based on the calculated energetic barrier for this process. Further, as the isopropyl group does not exert a significant effect on either the furyl-group rotation or the inversion of the helical chirality, the determined rotational barrier is also reflective of the barrier in the methyl-furyl fugid.



**Figure S3.** 2D- $^1\text{H}$ , $^1\text{H}$ -NOESY experiment of **1E** acquired at 600 MHz , mixing time  $d_8= 1.5\text{s}$

**Table S2.** NOE intensities and estimated (averaged) distances based on a two-spin approximation and calibration of distances using the fixed proton distances between furyl-H and methyl, and the isopropyliden methyl groups.

Protons	Protons	relative NOE intensity	distance (Å)	measured distance in $E_\alpha$ (Å)	measured distance in $E_\beta$ (Å)	
12-H	3-H	35.2	2.92	3.06	3.79	
12-H	15-H	20.3	3.20	4.52	3.39	
3-H	11-H	26.0	3.08	2.56	2.56	Fixed distance
3-H	14-H	12.8	3.46	3.67	3.36	
15-H	13-H	12.3	3.48	4.41	6.86	
15-H	14-H	19.7	3.22	4.02	4.46	
13-H	14-H	78.2	2.56	2.56	2.56	Calibration distance

The NOE intensity-derived distances were shorter than expected for the conformers **1E $_\alpha$**  or **1E $_\beta$**  alone and indicate a fast rotation and averaging over the conformers. This confirms the above statement of a fast thermal enantiotopomerisation that leads to a thermal equilibrium of both conformers in solution.

## 2. Quantum Chemical Calculations

Quantum chemical calculations were carried out using the Turbomole package. The ground state equilibrium structures of  $1E_{\alpha}$  and  $1E_{\beta}$  were calculated by DFT calculations at the B3LYP/def2-SVP level; the excited state structures are the results of a TDDFT geometry optimization with the same functional and basis set. The structural parameters are given in Table S3.

**Table S3.** Atomic cartesian coordinates (Å) of the calculated ground state equilibrium structures of  $1E_{\alpha}$  ( $1E_{\alpha \text{ eq}}$ ,  $1E_{\alpha \text{ FC}}^*$ ).

	x	y	z
C	2.257664	1.565058	-0.066287
C	1.001996	0.785992	-0.258485
C	1.425853	-0.627503	-0.236525
C	2.769183	-0.624164	0.403210
O	3.228380	0.686590	0.403838
C	-0.232561	1.361911	-0.239603
C	-0.436834	2.844498	-0.421217
C	0.931662	-1.701714	-0.897650
C	1.549519	-3.068870	-0.835054
O	3.454019	-1.497224	0.848038
O	2.523917	2.722378	-0.203739
C	-1.471872	0.622109	0.010453
C	-2.737584	0.832294	-0.653990
C	-3.644704	0.027447	-0.055995
O	-3.036174	-0.655096	0.964883
C	-1.721955	-0.288338	1.002825
C	-5.086238	-0.242909	-0.275822
H	-2.928595	1.486203	-1.487851
H	0.494693	3.389943	-0.506535
H	-1.020098	3.014708	-1.331062
H	-1.028442	3.247152	0.403451
H	1.902351	-3.358588	-1.829561
H	2.368971	-3.142583	-0.130900
H	0.779676	-3.798139	-0.563616
H	-5.456076	0.368023	-1.097451
H	-5.262665	-1.292533	-0.521927
H	-5.673073	-0.011666	0.615953
C	-0.258976	-1.612251	-1.802573
H	-1.169434	-1.923672	-1.282004
H	-0.427734	-0.604871	-2.174941
H	-0.128487	-2.288631	-2.649142
H	-0.559710	-1.880126	1.849916
C	-0.914212	-0.875809	2.098108
H	-1.510875	-0.948467	3.008032
H	-0.040426	-0.260433	2.301633

**Table S4.** Atomic cartesian coordinates (Å) of the calculated ground state equilibrium structures of  $1E_{\beta}$  ( $1E_{\beta \text{ eq}}$ ,  $1E_{\beta \text{ FC}}^*$ ).

	x	y	z
C	2.297049	1.507361	0.228512
C	1.054148	0.751937	-0.086148
C	1.476595	-0.655250	-0.214247
C	2.825685	-0.716821	0.430195
O	3.272435	0.586172	0.584485
C	-0.182909	1.343347	-0.013339
C	-0.312171	2.851869	0.051038
C	0.975476	-1.663294	-0.987328
C	1.568900	-3.046101	-1.021147
O	3.519515	-1.637726	0.756206
O	2.523731	2.684128	0.265847
C	-1.418160	0.560032	0.145726
C	-1.590644	-0.595260	1.002375
C	-2.904719	-0.949563	0.937105
O	-3.556234	-0.105194	0.079624
C	-2.667403	0.809847	-0.389935
C	-3.721025	-2.006633	1.593064
H	-0.824738	-1.068467	1.612023
H	0.265195	3.255962	0.897896
H	0.110678	3.337309	-0.842161
H	-1.358897	3.155420	0.172441
H	1.962077	-3.263240	-2.030854
H	2.367225	-3.192415	-0.287286
H	0.769404	-3.787326	-0.840923
H	-4.183723	-2.678291	0.849782
H	-3.090169	-2.610691	2.259734
H	-4.538288	-1.568791	2.191076
C	-0.185444	-1.461032	-1.919586
H	-0.013446	-2.023522	-2.852304
H	-1.118645	-1.851307	-1.476797
H	-0.352045	-0.404727	-2.164418
H	-3.906541	2.496421	-0.907283
C	-3.203487	1.787021	-1.378148
H	-3.757261	1.262540	-2.174478
H	-2.394557	2.363411	-1.844321



**Table S5.** Atomic cartesian coordinates (Å) of the calculated ground state equilibrium structures of  $1Z_{\alpha}$  ( $1Z_{\alpha,eq}$ ,  $1Z_{\alpha}^*$ ,  $1Z_{\alpha,FC}$ ).

	x	y	z
C	0.600140	1.560918	0.060126
C	0.780826	0.081635	-0.033245
C	2.238452	-0.135804	-0.039115
C	2.826814	1.143764	0.468342
O	1.830018	2.101415	0.430108
C	-0.244009	-0.803203	0.191129
C	0.023762	-2.231265	0.597329
C	2.982056	-1.118185	-0.626866
C	4.485303	-1.164254	-0.557106
O	3.935402	1.431995	0.820490
O	-0.357954	2.265425	-0.059564
C	-1.659838	-0.420844	0.050708
C	-2.252096	0.246518	-1.087226
C	-3.589836	0.328132	-0.852998
O	-3.866540	-0.230160	0.367302
C	-2.710349	-0.687146	0.910288
C	-4.738573	0.885287	-1.616102
H	-1.724782	0.615371	-1.963201
H	1.050404	-2.378063	0.956932
H	-0.672936	-2.532212	1.393144
H	-0.157830	-2.927694	-0.239112
H	4.906354	-0.433790	0.140204
H	4.807737	-2.178887	-0.263089
H	4.913849	-0.987501	-1.560593
H	-4.385779	1.315109	-2.563957
H	-5.489161	0.109148	-1.843697
H	-5.248976	1.680276	-1.046318
C	2.366003	-2.200668	-1.470290
H	2.332838	-3.165553	-0.933799
H	1.347101	-1.955531	-1.796574
H	2.990415	-2.367052	-2.364059
H	-1.857013	-1.303287	2.785175
C	-2.830149	-1.269933	2.277835
H	-3.247711	-2.292418	2.257955
H	-3.509839	-0.653231	2.887203

**Table S6.** Atomic cartesian coordinates (Å) of the calculated ground state equilibrium structures of  $1Z_{\beta}$  ( $1Z_{\beta \text{ eq}}$ ,  $1Z_{\beta \text{ FC}}^*$ ).

	x	y	z
C	0.733724	0.539999	-1.432762
C	0.772917	0.165311	0.011928
C	2.201842	0.003439	0.335328
C	2.887180	-0.140505	-0.987754
O	1.991721	0.260236	-1.962550
C	-0.339897	-0.249777	0.699405
C	-0.224904	-1.082116	1.952656
C	2.871243	0.215209	1.506086
O	3.999047	-0.475804	-1.282934
O	-0.143249	0.941588	-2.138503
C	-1.707240	0.083963	0.263939
C	-2.197703	1.401439	-0.075292
C	-3.528201	1.280117	-0.332980
O	-3.894351	-0.032593	-0.192806
C	-2.804645	-0.753195	0.171965
C	-4.594277	2.238569	-0.729541
H	-1.610382	2.314707	-0.119933
H	-0.978014	-1.883306	1.943435
H	0.768135	-1.536488	2.062881
H	-0.437168	-0.480794	2.853236
H	-5.414430	2.262152	0.008481
H	-4.175768	3.251025	-0.814687
H	-5.035466	1.965271	-1.703233
H	-2.073904	-2.773779	0.244451
C	-3.021626	-2.222860	0.304898
H	-3.674177	-2.577963	-0.508480
H	-3.516086	-2.485868	1.257259
C	2.189147	0.740186	2.740467
C	4.356249	0.016432	1.652017
H	2.049647	-0.051881	3.497459
H	2.826892	1.507094	3.211249
H	1.208846	1.184995	2.526872
H	4.825590	-0.392127	0.751829
H	4.550545	-0.664366	2.500582
H	4.842839	0.973712	1.912594

**Table S7.** Atomic cartesian coordinates (Å) of the calculated ground state equilibrium structures of **1C** ( $1C_{eq}$ ,  $1C^*_{FC}$ ).

	x	y	z
C	2.646454	1.108158	0.066034
C	1.197067	0.752856	0.029421
C	1.111274	-0.600180	-0.036081
C	2.469073	-1.143789	-0.110964
O	3.369187	-0.064431	-0.009432
C	0.073676	1.653087	-0.031953
C	0.248137	3.123688	-0.291011
C	-0.200095	-1.347048	-0.186021
C	-0.166608	-2.753350	0.434776
O	2.871449	-2.261538	-0.247509
O	3.172686	2.176777	0.149887
C	-1.133180	1.029875	0.062873
C	-2.475137	1.447007	-0.196684
C	-3.267257	0.344594	-0.169715
O	-2.606012	-0.794874	0.133063
C	-1.239416	-0.425782	0.508325
C	-4.717912	0.194096	-0.435277
H	-2.811486	2.437706	-0.454649
H	0.835454	3.597008	0.497856
H	0.783102	3.308191	-1.226110
H	-0.717368	3.625172	-0.345600
H	0.515950	-3.390246	-0.124694
H	0.175638	-2.742194	1.468875
H	-1.163258	-3.197642	0.402341
H	-5.163238	1.150493	-0.702882
H	-4.883397	-0.517188	-1.248382
H	-5.226218	-0.201387	0.448099
C	-0.498304	-1.480609	-1.700644
H	-1.429726	-2.023885	-1.859010
H	-0.578382	-0.506162	-2.184612
H	0.307319	-2.036145	-2.181154
H	-1.464557	-1.472705	2.399118
C	-1.192274	-0.480649	2.042987
H	-1.898958	0.240980	2.453315
H	-0.197409	-0.231198	2.410681

**Table S8.** Atomic cartesian coordinates (Å) of the calculated first excited state equilibrium structures of **1C\***<sub>min</sub>.

	x	y	z
C	2.647903	1.111775	0.080121
C	1.243889	0.787934	-0.023180
C	1.098627	-0.593025	-0.136151
C	2.459859	-1.172439	-0.105876
O	3.337361	-0.120833	0.007122
C	0.079776	1.675657	-0.033662
C	0.244194	3.118989	-0.365992
C	-0.207348	-1.306653	-0.295943
C	-0.162162	-2.768253	0.182913
O	2.824129	-2.325115	-0.173970
O	3.241079	2.165959	0.200664
C	-1.138527	1.045906	0.163720
C	-2.472834	1.463280	-0.138994
C	-3.279612	0.349330	-0.090284
O	-2.604161	-0.755568	0.280292
C	-1.224782	-0.414071	0.564893
C	-4.722452	0.173707	-0.392799
H	-2.798788	2.456615	-0.441696
H	1.073101	3.543964	0.224188
H	0.564262	3.232036	-1.419510
H	-0.672869	3.703441	-0.209322
H	0.481805	-3.357814	-0.483142
H	0.257823	-2.866594	1.192759
H	-1.175849	-3.199619	0.174201
H	-5.187733	1.132743	-0.656253
H	-4.856315	-0.531321	-1.231842
H	-5.250751	-0.258070	0.474435
C	-0.661265	-1.285201	-1.778726
H	-1.641141	-1.780525	-1.875451
H	-0.739022	-0.260721	-2.171811
H	0.068297	-1.831836	-2.393782
H	-1.349587	-1.650558	2.353195
C	-1.041394	-0.633699	2.075426
H	-1.660202	0.084629	2.633830
H	0.011931	-0.487724	2.354113

**Table S9.** Atomic cartesian coordinates (Å) of the calculated excited state structures of 1E at the final point of a TDDFT geometry optimization (**1E\*<sub>CI</sub>**).

	x	y	z
C	2.599585	1.179833	0.092458
C	1.171029	0.810700	-0.196422
C	1.164809	-0.596653	-0.430939
C	2.484273	-1.102663	-0.068142
O	3.319552	0.025335	0.179861
C	0.033780	1.644752	-0.109811
C	0.040181	3.111450	-0.473898
C	-0.003436	-1.450012	-0.623099
C	0.025880	-2.873931	-0.153806
O	2.943328	-2.211779	0.002370
O	3.079437	2.267175	0.275667
C	-1.196476	0.976846	0.116889
C	-2.529482	1.317229	-0.322411
C	-3.344949	0.298808	0.038704
O	-2.636386	-0.650292	0.757184
C	-1.346436	-0.243193	0.854926
C	-4.775747	-0.007582	-0.215606
H	-2.829764	2.185181	-0.906728
H	1.070052	3.489179	-0.522907
H	-0.434630	3.285180	-1.457703
H	-0.521896	3.702541	0.267081
H	0.397102	-3.530419	-0.965282
H	0.696370	-3.035516	0.699237
H	-0.993583	-3.222464	0.092984
H	-5.237129	0.797590	-0.804226
H	-4.886146	-0.960203	-0.760381
H	-5.336495	-0.106416	0.729953
C	-0.779946	-1.221134	-1.901911
H	-1.855699	-1.438968	-1.783469
H	-0.659241	-0.204136	-2.295543
H	-0.411957	-1.923100	-2.677819
H	-0.061524	-1.710675	1.863040
C	-0.604835	-0.777264	2.047606
H	-1.337814	-0.974368	2.845972
H	0.109130	-0.029588	2.421689

**Table S10.** Atomic cartesian coordinates (Å) of the calculated first excited state equilibrium structures of  $1E_{\alpha}^*_{\min}$ .

	x	y	z
C	1.371801	1.797476	0.097555
C	0.867127	0.608783	-0.565438
C	1.666410	-0.512390	-0.101361
C	2.613030	0.066897	0.916544
O	2.440932	1.427014	0.935055
C	-0.358609	0.648658	-1.333502
C	-0.662338	1.812621	-2.241051
C	1.765713	-1.800436	-0.574064
C	2.677283	-2.841429	0.019515
O	3.436108	-0.454289	1.622703
O	0.981517	2.948264	0.104788
C	-1.468750	0.059030	-0.556122
C	-1.886475	-1.273814	-0.370230
C	-2.960113	-1.268766	0.510179
O	-3.230961	0.014838	0.905170
C	-2.330615	0.821325	0.303565
C	-3.828866	-2.327876	1.057790
H	-1.473112	-2.158363	-0.843331
H	0.119963	1.898310	-3.014277
H	-1.622813	1.671848	-2.766357
H	-0.682646	2.796980	-1.732979
H	3.428102	-3.161688	-0.727839
H	3.202062	-2.490957	0.913612
H	2.099174	-3.751002	0.270968
H	-3.532404	-3.311964	0.673947
H	-3.770543	-2.337432	2.160415
H	-4.884401	-2.137160	0.796937
C	1.035189	-2.259713	-1.807320
H	0.400008	-3.143394	-1.604307
H	0.423294	-1.464637	-2.257679
H	1.770835	-2.599458	-2.560294
H	-2.882967	2.439025	1.566275
C	-2.357823	2.257439	0.618502
H	-2.883926	2.812208	-0.181557
H	-1.329944	2.658005	0.644306

**Table S11.** Atomic cartesian coordinates (Å) of the calculated first excited state equilibrium structures of  $1E_{\beta}^*_{\min}$ .

	x	y	z
C	2.260729	1.625619	-0.025875
C	1.113756	0.770592	-0.313618
C	1.610016	-0.595735	-0.314093
C	2.999022	-0.512035	0.253775
O	3.358722	0.804404	0.319019
C	-0.203287	1.293434	-0.428561
C	-0.483987	2.778789	-0.254868
C	1.104954	-1.766866	-0.843583
O	3.768082	-1.375469	0.591889
O	2.399215	2.826666	0.002719
C	-1.364158	0.469608	-0.000047
C	-1.678598	0.018808	1.287277
C	-2.930200	-0.608640	1.238953
O	-3.436353	-0.512220	-0.021948
C	-2.513215	0.136299	-0.779007
C	-3.735336	-1.335374	2.234455
H	-1.050498	0.103149	2.171350
H	-0.429911	3.122950	0.800476
H	0.253356	3.378122	-0.802690
H	-1.488404	3.046233	-0.628176
H	-3.250155	-1.319188	3.218057
H	-4.741514	-0.887326	2.311863
H	-3.881218	-2.383314	1.917176
H	-1.980347	0.812279	-2.701804
C	-2.868480	0.453495	-2.166784
H	-3.634014	1.252444	-2.185997
H	-3.308536	-0.424038	-2.667653
C	-0.062014	-1.788589	-1.795942
C	1.736974	-3.119426	-0.643156
H	-0.342881	-0.779997	-2.125596
H	0.214995	-2.364642	-2.699223
H	-0.949638	-2.304513	-1.381425
H	2.133812	-3.512784	-1.599889
H	0.971984	-3.850193	-0.315502
H	2.555068	-3.104995	0.083429

**Table S12.** Atomic cartesian coordinates (Å) of the calculated first excited state equilibrium structures of  $1Z_{\alpha}^{* \text{min}}$ .

	x	y	z
C	0.395616	1.317565	-0.251827
C	0.769425	-0.046834	0.039991
C	2.221001	-0.099742	-0.042166
C	2.657521	1.322761	-0.207137
O	1.527047	2.103624	-0.404767
C	-0.212313	-0.996392	0.429974
C	0.018845	-2.214275	1.289143
C	3.103825	-1.156027	-0.159115
C	4.600923	-0.997738	-0.127541
O	3.743364	1.835574	-0.236747
O	-0.713153	1.844445	-0.327464
C	-1.629762	-0.644972	0.160121
C	-2.466586	-1.084420	-0.874821
C	-3.681709	-0.418197	-0.756343
O	-3.646957	0.402970	0.339406
C	-2.433217	0.277483	0.906344
C	-4.923052	-0.409969	-1.551625
H	-2.205399	-1.782965	-1.666092
H	1.008270	-2.171599	1.766058
H	-0.724737	-2.279048	2.107345
H	-0.039629	-3.183806	0.752834
H	4.923106	0.013474	0.138569
H	5.037295	-1.717824	0.591275
H	5.042889	-1.251507	-1.110920
H	-4.859157	-1.124436	-2.381913
H	-5.790968	-0.661209	-0.917699
H	-5.106985	0.600233	-1.957747
C	2.648082	-2.568162	-0.411938
H	2.758964	-3.215306	0.479014
H	1.605521	-2.622808	-0.747813
H	3.283278	-3.021546	-1.194367
H	-2.037816	2.105079	1.860178
C	-2.167117	1.043612	2.131325
H	-1.239259	0.693694	2.598740
H	-3.014360	0.964262	2.831182



**Table S13.** Atomic cartesian coordinates (Å) of the calculated first excited state equilibrium structures of  $1Z_{\beta}^*_{\min}$ .

	x	y	z
C	0.425998	-0.210215	-1.243513
C	0.661080	-0.112177	0.178294
C	2.102684	-0.186662	0.360637
C	2.653135	-0.519042	-0.991322
O	1.618376	-0.436567	-1.913332
C	-0.427707	-0.071611	1.089629
C	-0.408474	-0.545563	2.521036
C	2.919257	0.145616	1.424116
O	3.763458	-0.777436	-1.369703
O	-0.622227	-0.171678	-1.886401
C	-1.761547	0.250831	0.522017
C	-2.460663	1.465320	0.544956
C	-3.627655	1.302675	-0.193983
O	-3.700434	0.014790	-0.654650
C	-2.599512	-0.633443	-0.232236
C	-4.728208	2.206349	-0.575977
H	-2.133417	2.392429	1.009449
H	-1.253132	-1.230125	2.732601
H	0.511738	-1.108423	2.731669
H	-0.477068	0.259913	3.281081
H	-5.699510	1.789998	-0.257705
H	-4.592315	3.198070	-0.126818
H	-4.770130	2.310175	-1.674521
H	-1.616328	-2.493895	-0.042980
C	-2.474160	-2.058555	-0.568182
H	-2.304518	-2.154254	-1.653480
H	-3.401554	-2.598020	-0.314531
C	2.410655	0.872599	2.640060
C	4.403327	-0.107438	1.444892
H	2.360777	0.220837	3.533290
H	3.114359	1.684435	2.899034
H	1.420747	1.318617	2.484655
H	4.751438	-0.704755	0.596901
H	4.681892	-0.618344	2.386736
H	4.963712	0.847571	1.445839

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