Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Investigation of Different Photochemical Reactions of Avobenzone Derivatives by Ultrafast Transient Absorption Spectroscopy

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Scheme 1S. Synthetic Route of AB-Me.

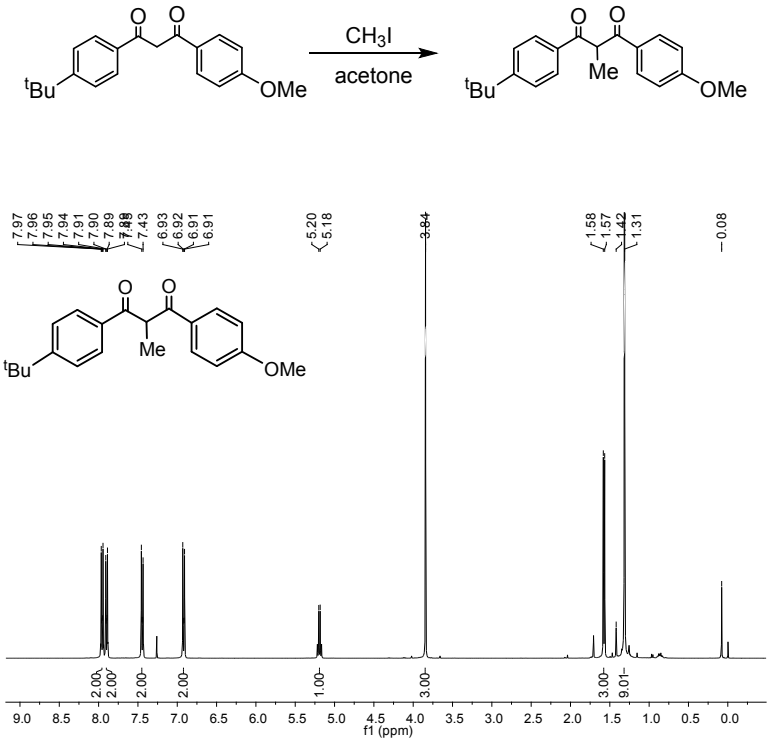


Figure 1S. The ^{1}H NMR spectra of AB-Me in $CDCl_3$.

Scheme 2S. Synthetic Route of AB-Pr.

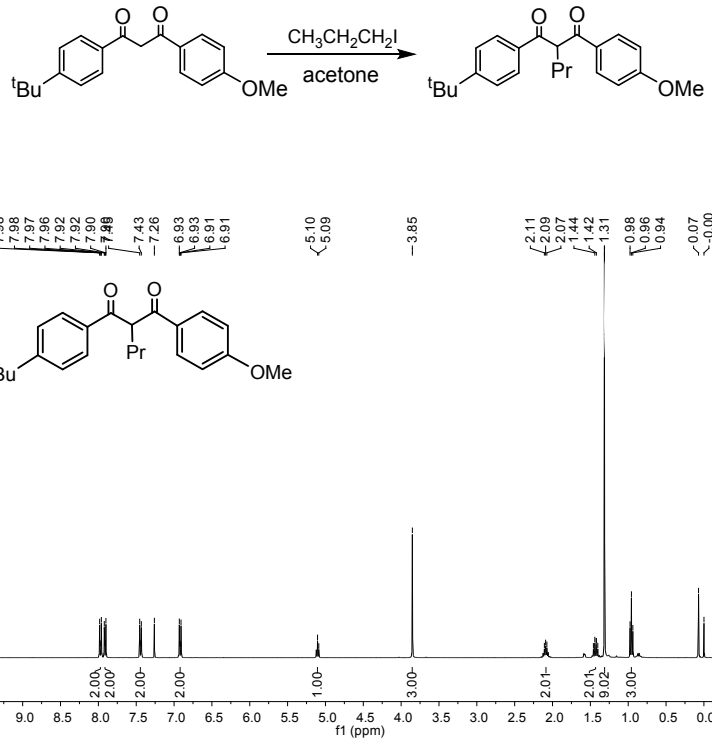
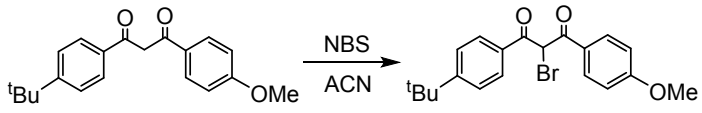


Figure 2S. The ^{1}H NMR spectra of AB-Pr in $CDCl_3$.

Scheme 3S. Synthetic Route of AB-Br.



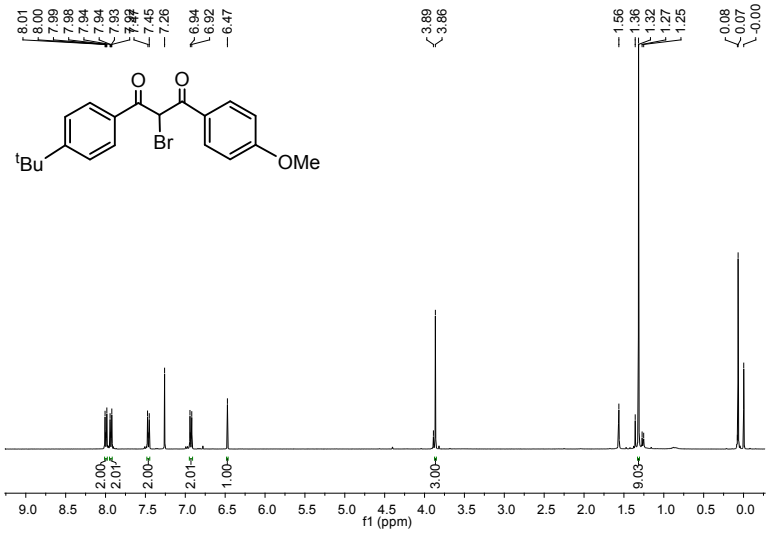
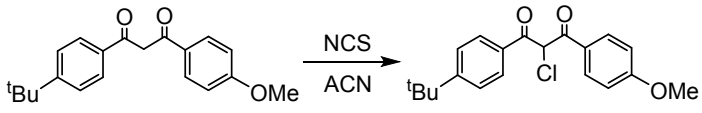


Figure 3S. The ^{1}H NMR spectra of AB-Br in $CDCl_3$.

Scheme 4S. Synthetic Route of AB-Cl



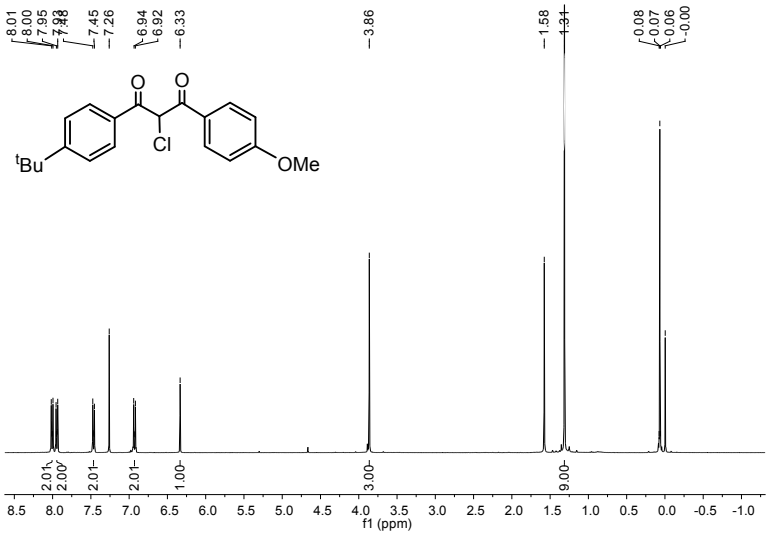


Figure 4S. The ^{1}H NMR spectra of AB-Br in $CDCl_3$.

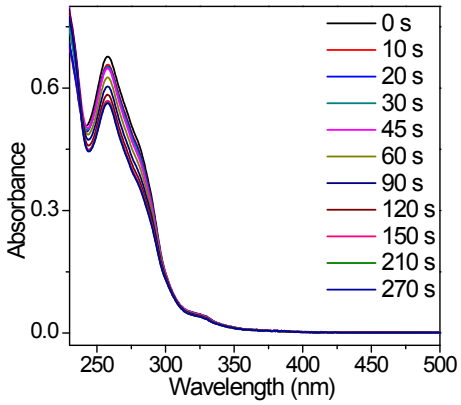


Figure 5S. Shown are UV-Vis absorption spectra of AB-Me in a N_2-purged ACN.

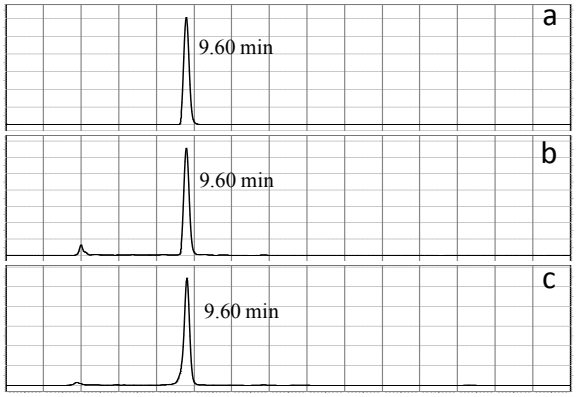


Figure 6S. HPLC analysis of the crude product of AB-Me in (b) ACN and (c) MeOH upon 266nm irradiation after 15 min. Retention time is 9.60 min for (a) AB-Me.

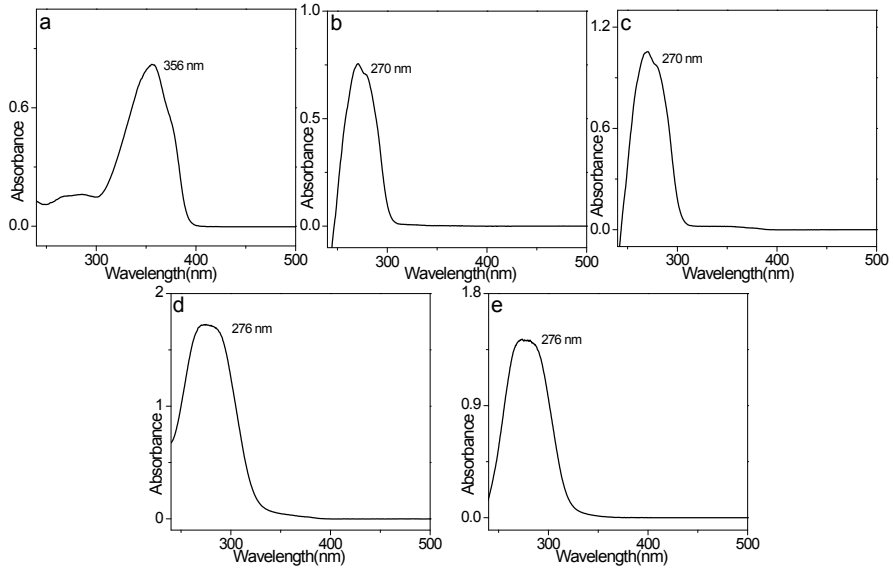


Figure 7S. Shown are UV-Vis absorption spectra of (a) AB (b) AB-Me (c) AB-Pr (d)AB-Br (e) AB-Cl in ACN.

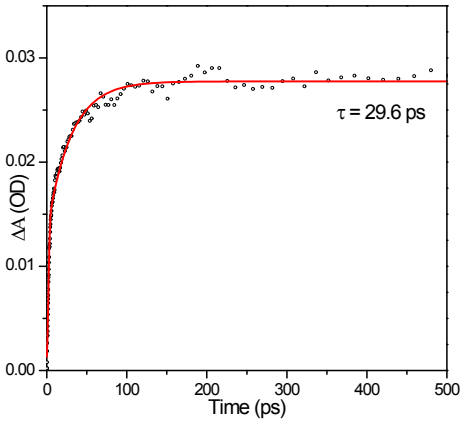


Figure 8S. Kinetic of the fs-TA bands observed at 410 nm of AB-Me. The solid lines indicate the kinetics fitting to the experimental data points.

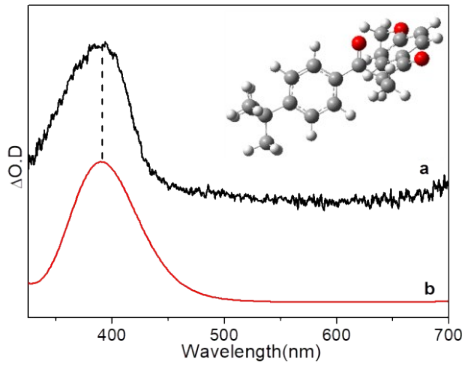


Figure 9S. The comparison of the computed electronic absorption spectrum of (AB-Me)^3 to the ns-TA spectrum recorded at 40 ns.

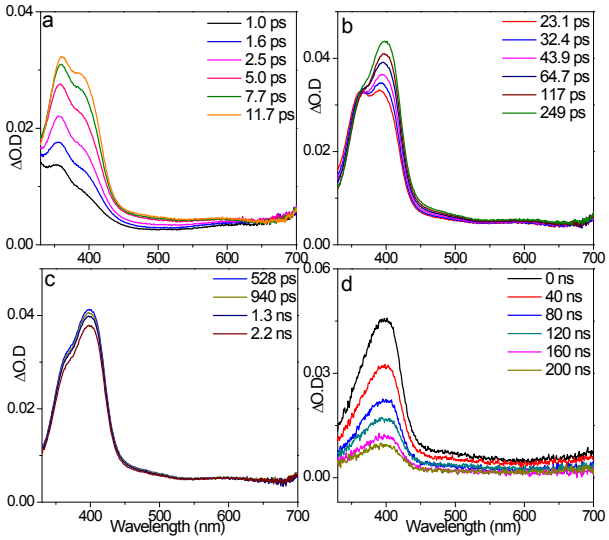


Figure 10S. (a-c) fs-TA and (d) ns-TA spectra of AB-Me in MeOH

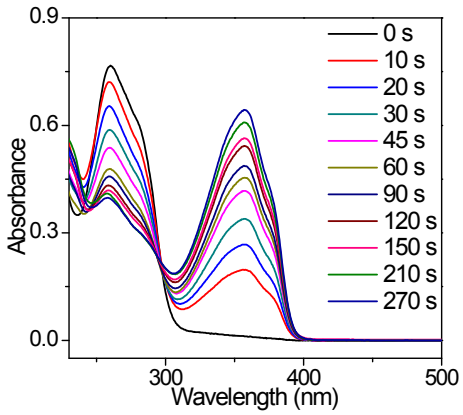


Figure 11S. Shown are UV-Vis absorption spectra of AB-Pr in ACN after irradiation for the specific time indicated in the figure.

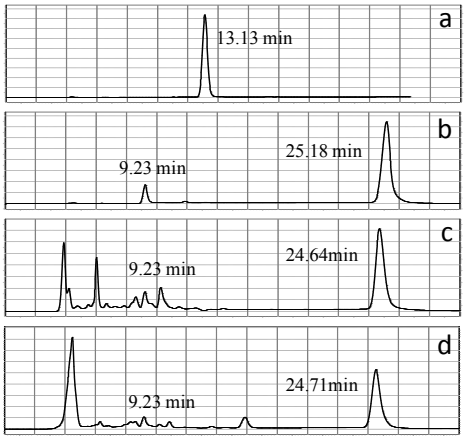


Figure 12S. HPLC analysis of the crude product of AB-Pr in (c) ACN and (d) MeOH upon 266 nm irradiation after 15 min. Retention times are (a) 13.13 min for AB-Pr and (b) 9.23 and 25.18 min for AB.

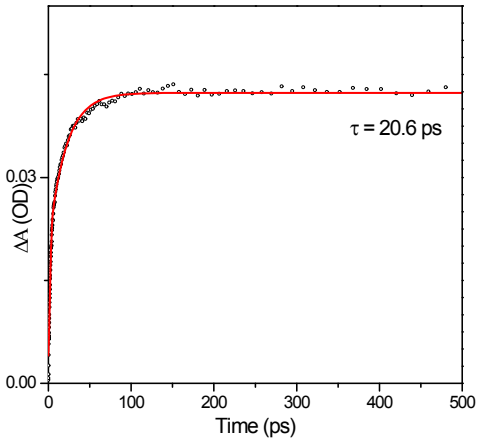


Figure 13S. Kinetic of the fs-TA bands observed at 410 nm of AB-Pr. The solid lines indicate the kinetics fitting to the experimental data points.

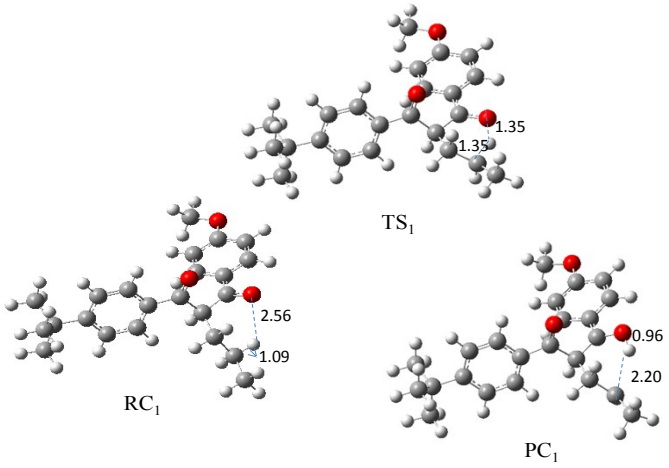
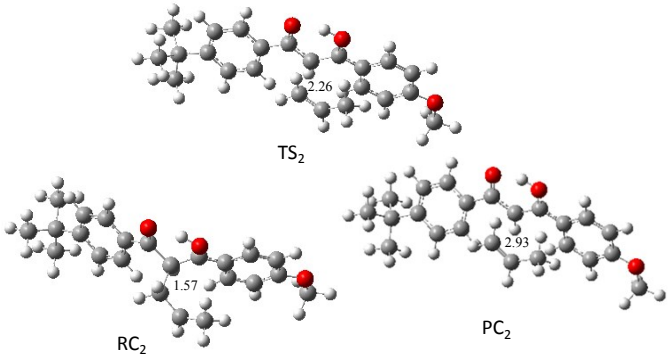


Figure 14S. Optimized geometries of RC_1, TS_1 and PC_1 obtained from (U)M06-2X/ 6-31G** calculations for the intramolecular hydrogen transfer of $(AB\text{-}Pr)^3$.



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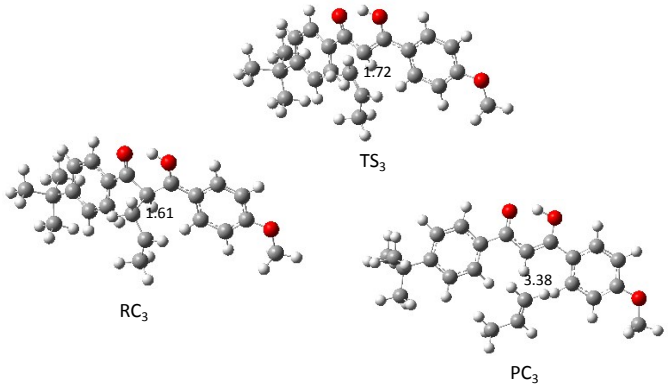


Figure 16S. Optimized geometries of RC_3, TS_3 and PC_3 obtained from (U)M06-2X/ 6-31G** calculations for the β-bond cleavage of open shell singlet biradical species.

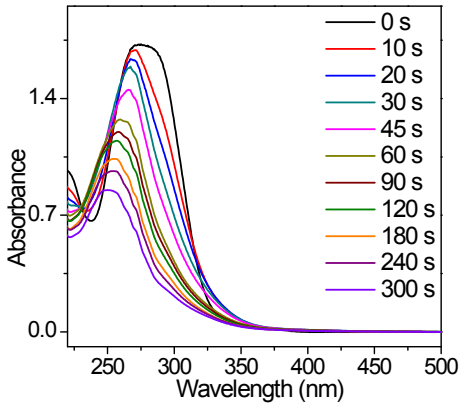


Figure 17S. Shown are UV-Vis absorption spectra of AB-Br in ACN after irradiation for the specific time indicated in the figure.

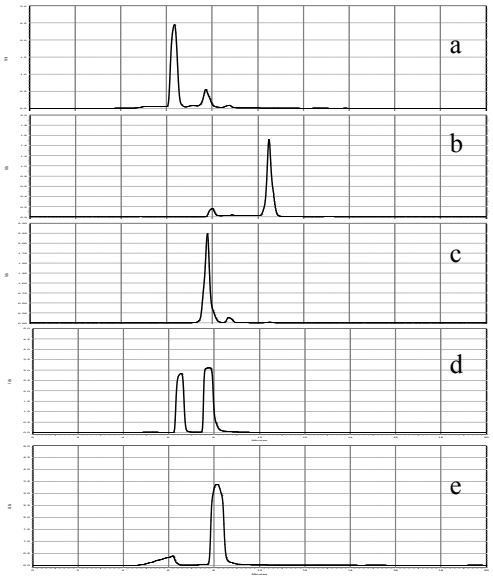


Figure 18S. HPLC analysis of the crude product of (a) AB-Br in ACN upon 266 nm irradiation after 15 min. Retention times are (b) 10.47 min for AB, (c) 7.78 min for AB-Br, (d) 6.53 and 7.72 min for *p*-methoxybenzoyl chloride upon 266 nm irradiation. (e) 8.14 min for *p* -tert-butylbenzaldehyde.

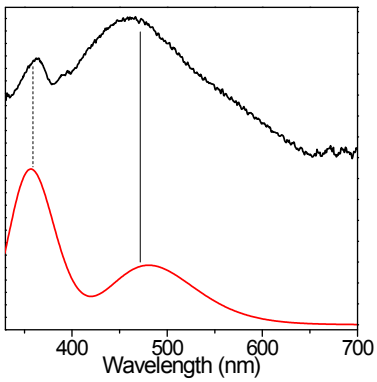


Figure 19S. Comparison of (black line) the second species derived from global fitting analysis for AB-Br in ACN with (red line) the calculated UV-Vis spectrum of $(AB\text{-}Br)^3$ obtained from (U)M06-2X/6-311+G** using a scale factor of 0.96.

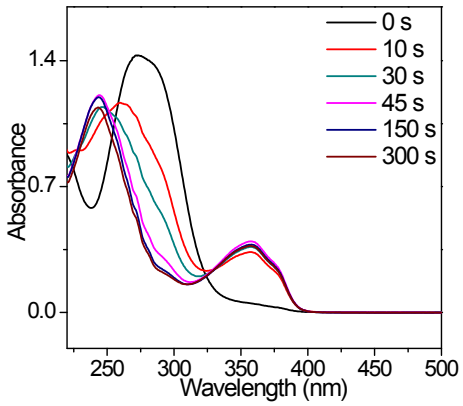


Figure 20S. Shown are UV-Vis absorption spectra of AB-Br in MeOH after irradiation for the specific time indicated in the figure.

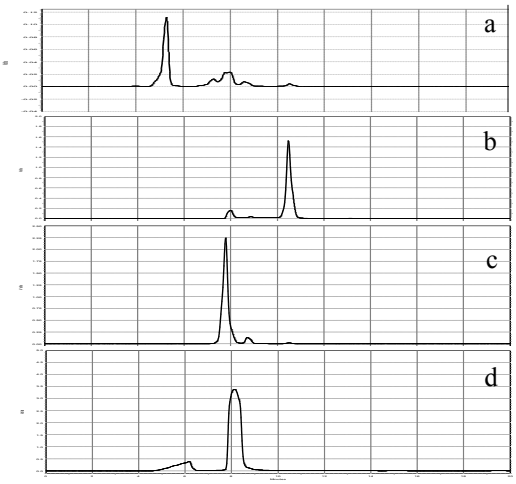


Figure 21S. HPLC analysis of the crude product of (a) AB-Br in MeOH upon 266 nm irradiation after 15 min. Retention times are (b) 10.47 min for AB, (c) 7.78 min for AB-Br, (d) 8.14 min for *p* -tert- butylbenzaldehyde.

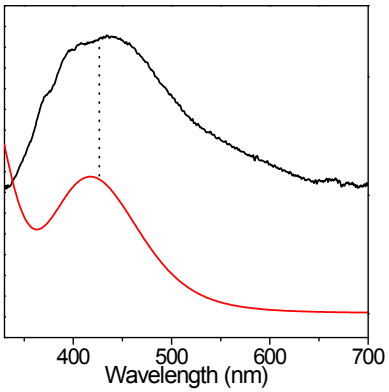


Figure 22S. Comparison of (black line) the second species derived from global fitting analysis for AB-Br in MeOH with (red line) the calculated UV-Vis spectrum of ketyl radical species with the structure inserted in the figure obtained from the (U)M06-2X/6-311+G** using a scale factor of 1.0.

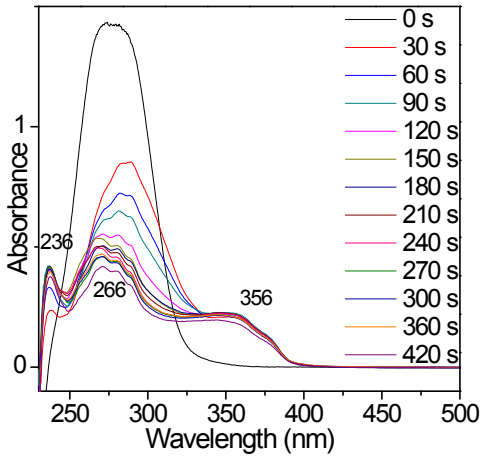


Figure 23S. Shown are UV-Vis absorption spectra of AB-Cl in ACN after irradiation for the specific time indicated in the figure.

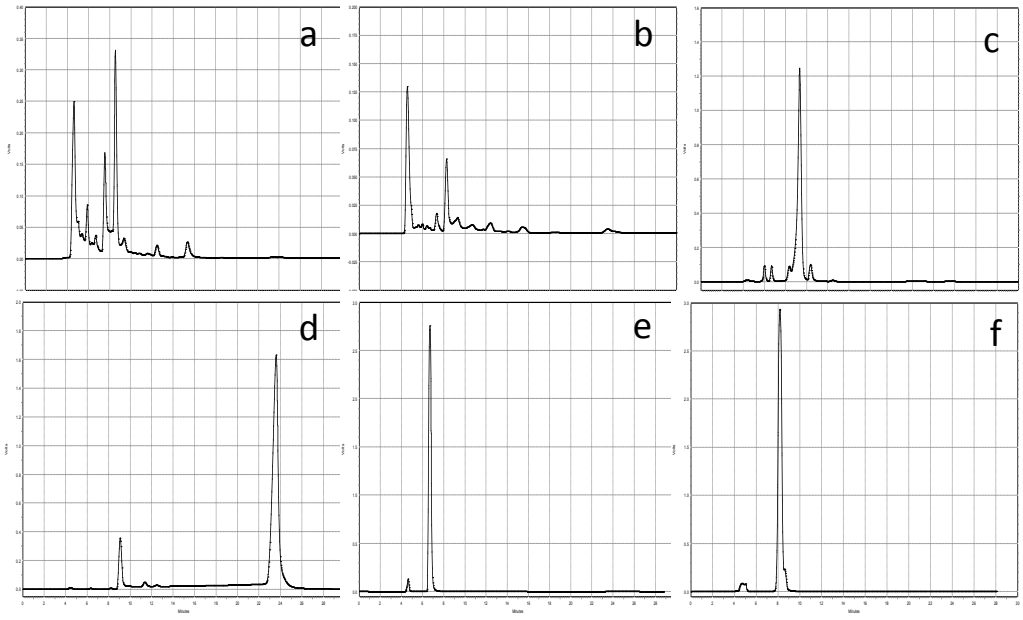


Figure 24S. HPLC analysis of the crude product of (a) AB-Cl in ACN and (b) AB-Cl in MeOH upon 266 nm irradiation after 15 min. Retention times are (c) 9.34 min for AB-Cl, (d) 9.08 and 23.6 min for AB, (e) 8.19 min for *p*-tert-butylbenzaldehyde, (f) 6.71 min for *p*-methoxybenzoyl chloride

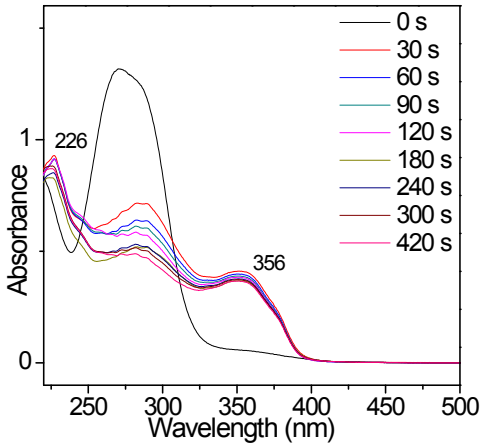


Figure 25S. Shown are UV-Vis absorption spectra of AB-Cl in MeOH after irradiation for the specific time indicated in the figure.

Table 1S. SOC (cm^{-1}) between the S_1 and T_2 states for AB-Me, AB-Pr, AB-Cl and AB-Br by using the BDF program.

	AB-Me	AB-Pr	AB-Cl	AB-Br
SOC (cm^{-1})	45.71	41.92	41.43	41.70

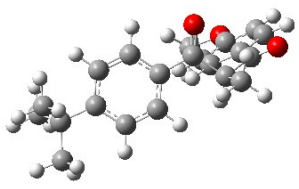
Table 2S. The transition configurations of the singlet and selected triplet excited states for AB-Me, AB-Pr, AB-Br and AB-Cl are given. H and L refer to HOMO and LUMO of the corresponding excited states, respectively.

	Transition configuration (%)	
Excited States	Matched	Others
AB-Me S_1（3.1922 eV）	H-3→L(20.9%)	H-5→L(45.0%) H-5→L+5(4.3%)
（f=0.0007）		H-4→L(14.6%)
AB-Me T_2（3.1859 eV）	H-3→L(6.4%)	H-9→L(5.3%) H-4→L+2(2.2%)
（f=0.0000）		H-1→L(77.8%)
AB-Pr S_1（3.1949 eV）	H-2→L(26.2%)	H-5→L+6(3.3%) H-5→L(337%)
（f=0.0009）		H-4→L(19.7%) H-2→L+6(2.3%)
AB-Pr T_2（3.1989 eV）	H-2→L(5.5%)	H-7→L(2.1%)
（f=0.0000）		H-1→L(78.8%)
AB-Cl S_1 (3.1368 eV)	H-7→L（7.9%）	H-5→L（50.0%）H-
(f=0.0009)	H-4→L（13.0%）	1→L+5（1.3%）
		H-3→L（1.4%）

AB-Cl T_2(3.1055 eV) (f=0.0000)	H-7→L（2.5%） H-4→L（2.1%）	H-13→L（6.3%）H-1→L（74.0%） H→L（2.1%）
AB-Br S_1 (3.0768 eV) (f=0.0011)	H-7→L(34.5%) H-4→L(33.3%) H-1→L(2.5%)	H-6→L(3.1%) H-5→L(8.0%) H-3→L(6.6%)
AB-Br T_2 (3.0914 eV) (f=0.0000)	H-7→L(5.0%) H-4→L(2.7%) H-1→L(67.2%)	H-13→L(5.3%) H-10→L(4.7%)

Cartesian coordinates, total energies, and vibrational zero-point energies for the optimized geometry for the compounds and intermediates considered in this paper are given.

Ground state of AB-Me:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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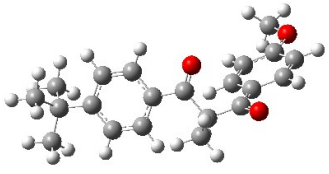
3	6	0	-3.046423	0.322670	1.252112
4	6	0	-3.686191	0.321690	0.003666
5	6	0	-3.049496	-0.335659	-1.048559
6	1	0	-1.362267	-1.464709	-1.712651
7	1	0	-1.340980	-0.306154	2.407129
8	1	0	-3.512834	0.822238	2.093798
9	1	0	-3.507353	-0.371140	-2.028177
10	6	0	-5.587493	0.912110	-1.575223
11	1	0	-6.543582	1.436917	-1.635196
12	1	0	-5.761395	-0.130723	-1.852569
13	1	0	-4.914440	1.360923	-2.310156
14	6	0	-4.852284	2.523799	0.173953
15	1	0	-4.498875	2.672841	1.196162
16	1	0	-5.806760	3.046303	0.066900
17	1	0	-4.129567	2.983199	-0.504921
18	6	0	-6.048080	0.410541	0.819201
19	1	0	-5.730086	0.516542	1.858138
20	1	0	-6.179477	-0.654237	0.612364
21	1	0	-7.017350	0.904850	0.711209
22	6	0	-5.031091	1.031623	-0.153346
23	6	0	-1.192672	-0.949806	0.375129
24	6	0	0.128576	-1.605393	0.641073
25	8	0	0.569675	-1.676508	1.762696
26	6	0	0.901131	-2.224444	-0.521335
27	1	0	0.695203	-1.676371	-1.444928
28	6	0	2.403253	-2.116156	-0.246688
29	8	0	3.076192	-3.108071	-0.113106
30	6	0	3.010286	-0.753303	-0.188647
31	6	0	4.384218	-0.652765	0.067583
32	6	0	2.279646	0.414882	-0.382043
33	6	0	5.002553	0.576435	0.129224
34	1	0	4.944357	-1.567437	0.218960

35	6	0	2.888853	1.664366	-0.322827
36	1	0	1.213507	0.379878	-0.580266
37	6	0	4.256838	1.746529	-0.064216
38	1	0	6.062043	0.673934	0.329661
39	1	0	2.292523	2.553073	-0.474348
40	6	0	4.238905	4.114742	-0.141012
41	1	0	3.788196	4.179851	-1.136263
42	1	0	4.971740	4.909196	-0.023026
43	1	0	3.460666	4.220200	0.621145
44	8	0	4.949697	2.903745	0.020280
45	6	0	0.475189	-3.687565	-0.668150
46	1	0	-0.596565	-3.762445	-0.862657
47	1	0	0.709423	-4.227341	0.249481
48	1	0	1.021776	-4.159918	-1.484101

Sum of electronic and zero-point Energies= -1039.784117

Sum of electronic and thermal Free Energies= -1039.837960

Triplet state of AB-Me:



Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z

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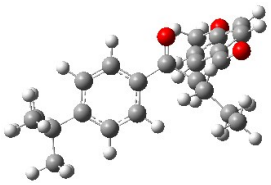
3	6	0	-3.086624	0.476887	1.213882
4	6	0	-3.769461	0.331875	-0.002950
5	6	0	-3.145265	-0.403460	-1.009629
6	1	0	-1.442899	-1.537087	-1.625098
7	1	0	-1.315713	0.029948	2.354027
8	1	0	-3.541910	1.038411	2.021964
9	1	0	-3.633732	-0.548696	-1.964111
10	6	0	-5.738947	0.712260	-1.562816
11	1	0	-6.718248	1.190801	-1.635569
12	1	0	-5.875968	-0.356485	-1.745684
13	1	0	-5.107542	1.123215	-2.354663
14	6	0	-5.017187	2.496364	0.015901
15	1	0	-4.647602	2.746888	1.012170
16	1	0	-5.992856	2.973341	-0.111691
17	1	0	-4.327090	2.920242	-0.717809
18	6	0	-6.107878	0.405203	0.880038
19	1	0	-5.758408	0.606068	1.894633
20	1	0	-6.209625	-0.676726	0.765204
21	1	0	-7.096603	0.858599	0.767670
22	6	0	-5.145603	0.975467	-0.175692
23	6	0	-1.216932	-0.812972	0.394037
24	6	0	0.144565	-1.383452	0.669849
25	8	0	0.654135	-1.246056	1.756562
26	6	0	0.859129	-2.162819	-0.432706
27	1	0	0.626770	-1.706519	-1.401748
28	6	0	2.373058	-2.112024	-0.230568
29	8	0	3.028655	-3.158256	-0.081195
30	6	0	3.023125	-0.842971	-0.250162
31	6	0	4.472620	-0.793048	-0.032827
32	6	0	2.323608	0.445409	-0.481965
33	6	0	5.112524	0.383777	0.046175
34	1	0	4.982745	-1.739138	0.082656
35	6	0	2.992232	1.619637	-0.392913
36	1	0	1.268118	0.449262	-0.721068
37	6	0	4.390926	1.635066	-0.106854
38	1	0	6.178908	0.449014	0.226236

39	1	0	2.459674	2.549099	-0.549549
40	6	0	4.515770	4.004284	-0.097437
41	1	0	4.083351	4.133926	-1.093156
42	1	0	5.299100	4.740907	0.059061
43	1	0	3.740076	4.122187	0.663745
44	8	0	5.142511	2.737480	0.017568
45	6	0	0.358992	-3.611343	-0.414410
46	1	0	-0.722254	-3.657805	-0.557712
47	1	0	0.613477	-4.070099	0.541387
48	1	0	0.853719	-4.184722	-1.197747

Sum of electronic and zero-point Energies= -1039.664773

Sum of electronic and thermal Free Energies= -1039.722923

Ground state of AB-Pr:



Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

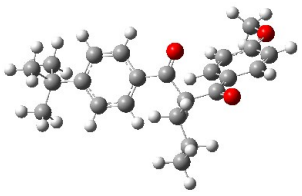
1	6	0	1.864645	0.617188	-0.614314
2	6	0	1.970047	-0.359337	1.575178
3	6	0	3.211202	-0.888732	1.276564
4	6	0	3.814068	-0.681032	0.026561
5	6	0	3.116715	0.083840	-0.907848
6	1	0	1.363619	1.215964	-1.366468
7	1	0	1.508883	-0.518698	2.542548
8	1	0	3.724709	-1.474499	2.030654
9	1	0	3.543836	0.277098	-1.882917
10	6	0	5.688901	-0.952347	-1.667086
11	1	0	6.670822	-1.406100	-1.820140
12	1	0	5.794030	0.125951	-1.811429
13	1	0	5.017367	-1.343072	-2.435862
14	6	0	5.102626	-2.816708	-0.125507
15	1	0	4.796051	-3.117269	0.878243
16	1	0	6.079217	-3.264770	-0.328305
17	1	0	4.381145	-3.225820	-0.837078
18	6	0	6.203090	-0.738918	0.759349
19	1	0	5.923381	-0.992688	1.783682
20	1	0	6.273602	0.349149	0.687225
21	1	0	7.192397	-1.162352	0.565622
22	6	0	5.188704	-1.286751	-0.258839
23	6	0	1.275804	0.399445	0.628591
24	6	0	-0.067875	0.940657	1.015869
25	8	0	-0.498916	0.786545	2.133186
26	6	0	-0.866878	1.734802	-0.012817
27	1	0	-0.692966	1.332096	-1.015616
28	6	0	-2.359714	1.591315	0.298222
29	8	0	-3.010204	2.538934	0.666595
30	6	0	-2.989003	0.251599	0.105482
31	6	0	-4.361252	0.126302	0.359972
32	6	0	-2.282815	-0.871079	-0.315536
33	6	0	-5.003620	-1.080599	0.193268
34	1	0	-4.902361	1.004103	0.691687
35	6	0	-2.916167	-2.098240	-0.486946
36	1	0	-1.217508	-0.817592	-0.514003
37	6	0	-4.283594	-2.204086	-0.233417

38	1	0	-6.062922	-1.195977	0.385070
39	1	0	-2.337396	-2.952456	-0.809577
40	6	0	-4.320191	-4.503801	-0.802987
41	1	0	-3.879576	-4.356910	-1.793993
42	1	0	-5.070899	-5.288743	-0.853399
43	1	0	-3.538082	-4.791866	-0.093716
44	8	0	-4.999267	-3.342317	-0.369871
45	6	0	-0.414434	3.201494	0.040490
46	1	0	0.679191	3.242278	0.096252
47	1	0	-0.805125	3.636364	0.964153
48	6	0	-0.892174	4.015693	-1.160034
49	1	0	-1.980197	3.944027	-1.229163
50	1	0	-0.480033	3.581384	-2.078613
51	6	0	-0.478019	5.480505	-1.050759
52	1	0	0.608652	5.576646	-0.976373
53	1	0	-0.915593	5.936738	-0.159783
54	1	0	-0.807545	6.054455	-1.918711

Sum of electronic and zero-point Energies= -1118.334220

Sum of electronic and thermal Free Energies= -1118.392035

Triplet state of AB-Pr:



Center	Atomic	Atomic	Coordinates (Angstroms)

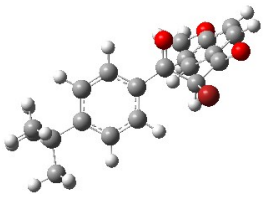
Number	Number	Type	X	Y	Z
1	6	0	1.939921	0.691093	-0.555344
2	6	0	1.878562	-0.603151	1.463434
3	6	0	3.135430	-1.103094	1.178977
4	6	0	3.831701	-0.717819	0.023668
5	6	0	3.208885	0.189364	-0.833025
6	1	0	1.497070	1.401363	-1.244563
7	1	0	1.345674	-0.898016	2.359491
8	1	0	3.586887	-1.806314	1.869900
9	1	0	3.708411	0.520779	-1.733708
10	6	0	5.831054	-0.755498	-1.545276
11	1	0	6.820305	-1.195731	-1.690868
12	1	0	5.950500	0.330459	-1.514703
13	1	0	5.219888	-1.014537	-2.413687
14	6	0	5.123345	-2.823984	-0.355712
15	1	0	4.734844	-3.268228	0.562813
16	1	0	6.112488	-3.250338	-0.544550
17	1	0	4.462161	-3.109965	-1.177351
18	6	0	6.157252	-0.921682	0.916943
19	1	0	5.799092	-1.325836	1.865836
20	1	0	6.233910	0.163533	1.019206
21	1	0	7.157946	-1.323263	0.735431
22	6	0	5.222615	-1.293054	-0.246715
23	6	0	1.260037	0.301476	0.595831
24	6	0	-0.112288	0.793380	0.959708
25	8	0	-0.615876	0.473885	2.009961
26	6	0	-0.844198	1.710922	-0.016306
27	1	0	-0.621913	1.383504	-1.039936
28	6	0	-2.354266	1.619076	0.206188
29	8	0	-3.013399	2.616408	0.553803
30	6	0	-2.998215	0.364168	-0.001857
31	6	0	-4.440967	0.268115	0.241277
32	6	0	-2.298120	-0.866715	-0.444858
33	6	0	-5.077874	-0.907865	0.129527
34	1	0	-4.950256	1.176940	0.529506
35	6	0	-2.964402	-2.041221	-0.548998
36	1	0	-1.242691	-0.829289	-0.680801

37	6	0	-4.359566	-2.109799	-0.254174
38	1	0	-6.139864	-1.008413	0.319252
39	1	0	-2.429981	-2.929720	-0.860883
40	6	0	-4.487025	-4.441924	-0.674067
41	1	0	-4.079282	-4.383709	-1.686769
42	1	0	-5.268235	-5.196315	-0.635897
43	1	0	-3.693311	-4.696432	0.033227
44	8	0	-5.108190	-3.219317	-0.312187
45	6	0	-0.339329	3.150989	0.169364
46	1	0	0.748194	3.150810	0.301819
47	1	0	-0.781246	3.541817	1.089625
48	6	0	-0.710445	4.057457	-1.002311
49	1	0	-1.794892	4.036250	-1.131445
50	1	0	-0.265378	3.658941	-1.922287
51	6	0	-0.242483	5.493111	-0.782330
52	1	0	0.842243	5.537772	-0.651471
53	1	0	-0.704657	5.913869	0.113790
54	1	0	-0.505934	6.132172	-1.627252

Sum of electronic and zero-point Energies= -1118.215084

Sum of electronic and thermal Free Energies= -1118.275204

Ground state of AB-Br:



Center	Atomic	Atomic	Coordinates (Angstroms)

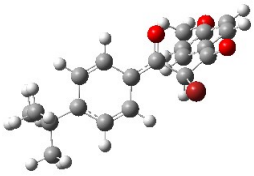
Number	Number	Type	X	Y	Z
1	6	0	-1.888787	-0.517427	-0.705301
2	6	0	-1.885434	0.401822	1.514719
3	6	0	-3.115679	0.982704	1.272541
4	6	0	-3.766463	0.830528	0.038953
5	6	0	-3.129311	0.067736	-0.939696
6	1	0	-1.443978	-1.126663	-1.483547
7	1	0	-1.388290	0.519260	2.470080
8	1	0	-3.582236	1.564842	2.058997
9	1	0	-3.597268	-0.087023	-1.902705
10	6	0	-5.687364	1.214763	-1.578842
11	1	0	-6.657632	1.705240	-1.684661
12	1	0	-5.834784	0.145477	-1.749958
13	1	0	-5.029529	1.605401	-2.359414
14	6	0	-4.984004	3.012116	-0.006124
15	1	0	-4.634306	3.272514	0.994735
16	1	0	-5.950884	3.498177	-0.161972
17	1	0	-4.273314	3.418260	-0.730146
18	6	0	-6.124341	0.946955	0.857940
19	1	0	-5.800614	1.160520	1.878461
20	1	0	-6.235141	-0.135458	0.757394
21	1	0	-7.104271	1.409216	0.711381
22	6	0	-5.127824	1.490495	-0.180180
23	6	0	-1.253159	-0.353668	0.522853
24	6	0	0.082541	-0.936557	0.844658
25	8	0	0.567534	-0.856422	1.943936
26	6	0	0.873311	-1.629846	-0.272689
27	1	0	0.688083	-1.169283	-1.241941
28	6	0	2.378589	-1.586926	0.032103
29	8	0	3.006817	-2.577517	0.284343
30	6	0	3.012806	-0.238228	-0.036812
31	6	0	4.387494	-0.152807	0.222412
32	6	0	2.317158	0.926987	-0.347869
33	6	0	5.040524	1.058286	0.170588
34	1	0	4.921456	-1.062844	0.466874
35	6	0	2.962692	2.157492	-0.404768
36	1	0	1.250678	0.909641	-0.547176

37	6	0	4.331550	2.225214	-0.144360
38	1	0	6.101139	1.143637	0.370062
39	1	0	2.392785	3.043444	-0.647043
40	6	0	4.388965	4.572169	-0.469638
41	1	0	3.951432	4.543290	-1.472298
42	1	0	5.146491	5.350797	-0.426638
43	1	0	3.607583	4.782752	0.266841
44	8	0	5.057768	3.362424	-0.170245
45	35	0	0.215316	-3.449998	-0.410701

Sum of electronic and zero-point Energies= -3574.081981

Sum of electronic and thermal Free Energies= -3574.137335

Triplet state of AB-Br:



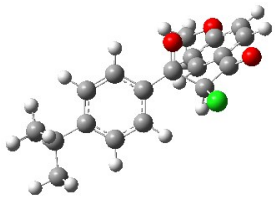
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.945761	-0.360781	-0.798523
2	6	0	-1.993558	0.538886	1.546284
3	6	0	-3.213669	1.047301	1.305951
4	6	0	-3.880904	0.898873	0.019335
5	6	0	-3.171138	0.164578	-1.003540
6	1	0	-1.461710	-0.927473	-1.582422
7	1	0	-1.499068	0.644075	2.502170
8	1	0	-3.725369	1.584600	2.096281

9	1	0	-3.641693	0.022752	-1.968043
10	6	0	-5.804992	1.239833	-1.586352
11	1	0	-6.793778	1.694387	-1.677616
12	1	0	-5.911075	0.170288	-1.784087
13	1	0	-5.165661	1.676479	-2.357778
14	6	0	-5.169117	3.025617	0.036863
15	1	0	-4.822770	3.273567	1.041997
16	1	0	-6.158088	3.471917	-0.097857
17	1	0	-4.483858	3.481040	-0.681938
18	6	0	-6.227612	0.893687	0.848039
19	1	0	-5.906613	1.083830	1.873926
20	1	0	-6.310106	-0.186990	0.711487
21	1	0	-7.219539	1.335078	0.718824
22	6	0	-5.252644	1.500891	-0.181562
23	6	0	-1.271364	-0.202205	0.503228
24	6	0	0.014495	-0.721854	0.816289
25	8	0	0.523318	-0.548274	1.941114
26	6	0	0.787569	-1.496182	-0.240020
27	1	0	0.705077	-1.034177	-1.224584
28	6	0	2.270779	-1.601371	0.146059
29	8	0	2.769751	-2.640930	0.478362
30	6	0	3.069908	-0.343869	0.039695
31	6	0	4.445303	-0.431291	0.293029
32	6	0	2.531465	0.891997	-0.305009
33	6	0	5.253280	0.679804	0.195670
34	1	0	4.855173	-1.395665	0.566837
35	6	0	3.333933	2.023996	-0.405727
36	1	0	1.468873	1.004352	-0.489313
37	6	0	4.702023	1.918244	-0.156210
38	1	0	6.317683	0.630365	0.387041
39	1	0	2.883722	2.970467	-0.670080
40	6	0	5.065837	4.222272	-0.573938
41	1	0	4.611527	4.207884	-1.569655
42	1	0	5.920604	4.894078	-0.575782
43	1	0	4.331069	4.569033	0.159237
44	8	0	5.572497	2.949235	-0.226524
45	35	0	-0.005198	-3.273734	-0.454846

Sum of electronic and zero-point Energies= -3573.963970

Sum of electronic and thermal Free Energies= -3574.020846

Ground state of AB-Cl:



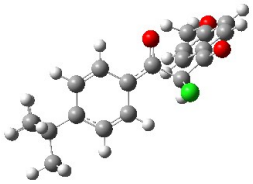
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893161	-0.843853	-0.765728
2	6	0	-1.865532	0.026727	1.474217
3	6	0	-3.092901	0.622074	1.253892
4	6	0	-3.753925	0.502305	0.022026
5	6	0	-3.131645	-0.245504	-0.977430
6	1	0	-1.458024	-1.438092	-1.560899
7	1	0	-1.360463	0.119055	2.428256
8	1	0	-3.549334	1.191059	2.055723
9	1	0	-3.608523	-0.376744	-1.939576
10	6	0	-5.680427	0.946305	-1.573882
11	1	0	-6.643886	1.453235	-1.662371
12	1	0	-5.844622	-0.116437	-1.768643
13	1	0	-5.021333	1.345461	-2.349055
14	6	0	-4.946742	2.697410	0.036520
15	1	0	-4.587387	2.930112	1.040812
16	1	0	-5.909041	3.197757	-0.101090

17	1	0	-4.236374	3.112572	-0.682693
18	6	0	-6.105231	0.625152	0.858984
19	1	0	-5.772680	0.810585	1.882197
20	1	0	-6.228942	-0.453194	0.733231
21	1	0	-7.080756	1.101625	0.729702
22	6	0	-5.109206	1.182045	-0.172558
23	6	0	-1.246153	-0.709952	0.460016
24	6	0	0.087549	-1.309404	0.752456
25	8	0	0.581566	-1.275024	1.849401
26	6	0	0.863037	-1.969070	-0.399899
27	1	0	0.681735	-1.456931	-1.344649
28	6	0	2.371701	-1.954732	-0.103858
29	8	0	2.983106	-2.967352	0.095034
30	6	0	3.025993	-0.615277	-0.115341
31	6	0	4.404353	-0.562714	0.132241
32	6	0	2.344149	0.573275	-0.361377
33	6	0	5.074583	0.640051	0.133046
34	1	0	4.926548	-1.491751	0.325490
35	6	0	3.006884	1.795876	-0.363905
36	1	0	1.275748	0.580554	-0.551071
37	6	0	4.379038	1.831036	-0.114231
38	1	0	6.138247	0.700449	0.325106
39	1	0	2.448554	2.701122	-0.556009
40	6	0	4.462806	4.191802	-0.301430
41	1	0	4.013382	4.232902	-1.298404
42	1	0	5.229723	4.957781	-0.217795
43	1	0	3.692400	4.363020	0.456474
44	8	0	5.120780	2.958277	-0.088035
45	17	0	0.249435	-3.631333	-0.590499

Sum of electronic and zero-point Energies= -1460.106713

Sum of electronic and thermal Free Energies= -1460.161186

Triplet state of AB-Cl:



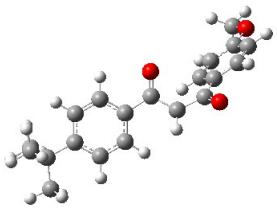
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.980330	-0.766980	-0.844139
2	6	0	-1.996704	0.076794	1.522518
3	6	0	-3.204504	0.621094	1.299480
4	6	0	-3.873137	0.534201	0.008345
5	6	0	-3.192088	-0.205926	-1.031649
6	1	0	-1.520813	-1.344282	-1.635288
7	1	0	-1.500249	0.137882	2.481239
8	1	0	-3.705459	1.141834	2.107621
9	1	0	-3.676847	-0.326030	-1.992126
10	6	0	-5.776028	0.999784	-1.591782
11	1	0	-6.741699	1.503043	-1.673665
12	1	0	-5.931642	-0.056829	-1.823399
13	1	0	-5.111412	1.429260	-2.345665
14	6	0	-5.084235	2.703469	0.095071
15	1	0	-4.728310	2.903725	1.107555
16	1	0	-6.057045	3.188597	-0.021846
17	1	0	-4.384011	3.159462	-0.608802
18	6	0	-6.222792	0.584457	0.827882
19	1	0	-5.902988	0.732344	1.861065
20	1	0	-6.339023	-0.488189	0.657097
21	1	0	-7.199240	1.061135	0.706455
22	6	0	-5.221598	1.191344	-0.176579
23	6	0	-1.283815	-0.629172	0.448145
24	6	0	0.017478	-1.130990	0.718642
25	8	0	0.544168	-0.990004	1.839683
26	6	0	0.787977	-1.844351	-0.387068

27	1	0	0.686790	-1.325636	-1.342510
28	6	0	2.280805	-1.935961	-0.029153
29	8	0	2.801255	-2.986707	0.225360
30	6	0	3.054607	-0.660378	-0.063812
31	6	0	4.433459	-0.737408	0.172863
32	6	0	2.489673	0.584310	-0.323811
33	6	0	5.219201	0.393311	0.144890
34	1	0	4.864371	-1.709722	0.377905
35	6	0	3.269472	1.736285	-0.353521
36	1	0	1.423906	0.687274	-0.495142
37	6	0	4.640952	1.641421	-0.118373
38	1	0	6.285852	0.352286	0.325341
39	1	0	2.799411	2.689472	-0.551173
40	6	0	4.954608	3.975987	-0.374662
41	1	0	4.495163	4.024372	-1.366908
42	1	0	5.794514	4.664908	-0.330634
43	1	0	4.216319	4.251850	0.384710
44	8	0	5.490000	2.692503	-0.121959
45	17	0	0.098295	-3.481814	-0.648601

Sum of electronic and zero-point Energies= -1459.988858

Sum of electronic and thermal Free Energies= -1460.045303

The radical species of photodebromination and photodechlorination



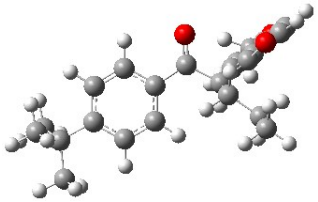
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.106435	-0.764197	-0.841151
2	6	0	-2.158110	0.284479	1.317049
3	6	0	-3.493217	0.591355	1.131761
4	6	0	-4.170528	0.234261	-0.043775
5	6	0	-3.447775	-0.442148	-1.026238
6	1	0	-1.577555	-1.279498	-1.635072
7	1	0	-1.636845	0.570529	2.222611
8	1	0	-4.021707	1.120138	1.917103
9	1	0	-3.923638	-0.728423	-1.954684
10	6	0	-6.220351	0.122426	-1.541140
11	1	0	-7.275792	0.397809	-1.601196
12	1	0	-6.152443	-0.963164	-1.649015
13	1	0	-5.705396	0.589913	-2.384307
14	6	0	-5.811010	2.119645	-0.113032
15	1	0	-5.457121	2.509249	0.843591
16	1	0	-6.865549	2.389327	-0.217247
17	1	0	-5.248897	2.614257	-0.908962
18	6	0	-6.450556	-0.074522	0.929586
19	1	0	-6.121953	0.267229	1.912945
20	1	0	-6.337730	-1.160789	0.893561
21	1	0	-7.512147	0.165694	0.826455
22	6	0	-5.648412	0.592733	-0.200611
23	6	0	-1.449420	-0.409177	0.333077
24	6	0	-0.003018	-0.701170	0.580722
25	8	0	0.605554	-0.133478	1.474855
26	6	0	0.650884	-1.719207	-0.238258
27	1	0	0.047700	-2.447817	-0.765495
28	6	0	2.089613	-2.074281	-0.168259
29	8	0	2.354582	-3.262321	-0.177262
30	6	0	3.148873	-1.038028	-0.119269
31	6	0	4.454011	-1.443428	0.189192
32	6	0	2.913820	0.296699	-0.432251
33	6	0	5.486831	-0.532495	0.205686
34	1	0	4.630364	-2.487726	0.416463
35	6	0	3.947922	1.225035	-0.434004

36	1	0	1.915615	0.630455	-0.686998
37	6	0	5.239624	0.811274	-0.105414
38	1	0	6.500393	-0.821170	0.453619
39	1	0	3.735260	2.255114	-0.683505
40	6	0	6.118424	2.997953	-0.354539
41	1	0	5.750359	3.136896	-1.375712
42	1	0	7.093857	3.467507	-0.253680
43	1	0	5.418768	3.453767	0.352613
44	8	0	6.314543	1.627982	-0.064829

Sum of electronic and zero-point Energies= -999.861890

Sum of electronic and thermal Free Energies= -999.914917

The reaction complex of the intramolecular hydrogen transfer of (AB-Pr)^3



Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z

1	6	0	1.908038	0.534303	-0.632778
2	6	0	2.170821	-0.197900	1.641363
3	6	0	3.398911	-0.748025	1.319342
4	6	0	3.918023	-0.669525	0.016845

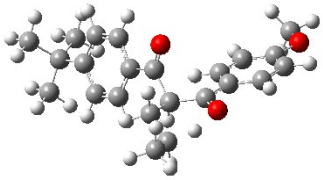
5	6	0	3.149256	-0.015296	-0.947692
6	1	0	1.349103	1.040145	-1.414571
7	1	0	1.772837	-0.256623	2.649019
8	1	0	3.969096	-1.249847	2.095917
9	1	0	3.511163	0.074672	-1.965228
10	6	0	5.684895	-1.107388	-1.756897
11	1	0	6.662957	-1.567153	-1.925841
12	1	0	5.763583	-0.048565	-2.022858
13	1	0	4.970240	-1.583989	-2.435228
14	6	0	5.228354	-2.798721	0.012713
15	1	0	4.986655	-2.990674	1.061569
16	1	0	6.199377	-3.258538	-0.198236
17	1	0	4.471835	-3.292489	-0.604540
18	6	0	6.350695	-0.628108	0.593488
19	1	0	6.136721	-0.763942	1.657029
20	1	0	6.406733	0.446213	0.394185
21	1	0	7.332175	-1.068350	0.389250
22	6	0	5.281416	-1.291648	-0.290964
23	6	0	1.404440	0.449193	0.665196
24	6	0	0.083452	1.017659	1.085684
25	8	0	-0.257013	1.009481	2.248229
26	6	0	-0.821861	1.653162	0.017456
27	1	0	-0.667476	1.151690	-0.945045
28	6	0	-2.272788	1.453663	0.373464
29	8	0	-2.841240	2.463252	1.020377
30	6	0	-2.994197	0.244162	0.182718
31	6	0	-4.375865	0.161156	0.504002
32	6	0	-2.370363	-0.916541	-0.324498
33	6	0	-5.079601	-1.005055	0.307560
34	1	0	-4.881611	1.034689	0.903725
35	6	0	-3.085583	-2.090009	-0.525245
36	1	0	-1.307200	-0.913153	-0.546486
37	6	0	-4.445917	-2.143735	-0.213255
38	1	0	-6.135262	-1.071682	0.548200
39	1	0	-2.568407	-2.958913	-0.914562
40	6	0	-4.621962	-4.411149	-0.862593
41	1	0	-4.206192	-4.254948	-1.865776
42	1	0	-5.403274	-5.169340	-0.911123

43	1	0	-3.822689	-4.755066	-0.194356
44	8	0	-5.234912	-3.241873	-0.371090
45	6	0	-0.428666	3.135975	-0.132734
46	1	0	0.653901	3.188532	-0.305971
47	1	0	-0.617316	3.645779	0.819913
48	6	0	-1.163575	3.845660	-1.268254
49	1	0	-2.242559	3.795438	-1.087507
50	1	0	-0.976342	3.309925	-2.207786
51	6	0	-0.726865	5.301449	-1.405262
52	1	0	0.346892	5.372861	-1.605452
53	1	0	-0.931357	5.856389	-0.484702
54	1	0	-1.254628	5.800346	-2.221617

Sum of electronic and zero-point Energies= -1117.951702

Sum of electronic and thermal Free Energies= -1118.009520

The transition state of the intramolecular hydrogen transfer of (AB-Pr)^3



Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms) X	Y	Z
1	6	0	-1.835850	0.858997	0.735740
2	6	0	-1.954421	-0.051703	-1.484642
3	6	0	-3.235603	-0.505958	-1.227463
4	6	0	-3.853832	-0.290369	0.015235
5	6	0	-3.129636	0.404858	0.985103
6	1	0	-1.314661	1.397046	1.520935
7	1	0	-1.480066	-0.216034	-2.446465
8	1	0	-3.769563	-1.040699	-2.007924

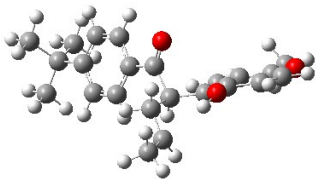
9	1	0	-3.567301	0.599992	1.957208
10	6	0	-5.781083	-0.481908	1.660558
11	1	0	-6.791593	-0.881857	1.785180
12	1	0	-5.827477	0.599552	1.822597
13	1	0	-5.150111	-0.923206	2.438473
14	6	0	-5.264209	-2.350870	0.098583
15	1	0	-4.955435	-2.650712	-0.906589
16	1	0	-6.268798	-2.748702	0.275698
17	1	0	-4.579009	-2.813155	0.815433
18	6	0	-6.227421	-0.201834	-0.772812
19	1	0	-5.936444	-0.451630	-1.796729
20	1	0	-6.244742	0.888306	-0.681873
21	1	0	-7.243074	-0.577512	-0.610914
22	6	0	-5.267992	-0.820812	0.257777
23	6	0	-1.231454	0.634737	-0.501100
24	6	0	0.149291	1.095626	-0.858812
25	8	0	0.553876	1.001493	-1.996641
26	6	0	1.032767	1.767667	0.207090
27	1	0	0.662543	1.523621	1.212542
28	6	0	2.474606	1.316645	0.095234
29	8	0	3.461119	2.228404	0.064959
30	6	0	2.865063	-0.055140	0.101521
31	6	0	4.232732	-0.419900	-0.018038
32	6	0	1.929938	-1.101755	0.252300
33	6	0	4.622119	-1.740276	-0.002209
34	1	0	4.976567	0.361814	-0.126214
35	6	0	2.324890	-2.433998	0.271881
36	1	0	0.873714	-0.884037	0.380257
37	6	0	3.673962	-2.764687	0.139099
38	1	0	5.666174	-2.019418	-0.097720
39	1	0	1.569832	-3.201371	0.394618
40	6	0	3.238814	-5.086380	0.269026
41	1	0	2.696566	-5.029532	1.221416
42	1	0	3.815616	-6.010596	0.238285
43	1	0	2.513323	-5.083254	-0.554125
44	8	0	4.166876	-4.035328	0.140755
45	6	0	0.903683	3.280381	-0.036443
46	1	0	-0.110754	3.608964	0.229431

47	1	0	1.038894	3.464868	-1.108432
48	6	0	1.945808	4.054686	0.734984
49	1	0	2.923956	3.404739	0.458948
50	1	0	1.858182	3.920400	1.818739
51	6	0	2.154268	5.493279	0.320059
52	1	0	1.249428	6.078345	0.525696
53	1	0	2.360046	5.564608	-0.751241
54	1	0	2.980574	5.955188	0.864175

Sum of electronic and zero-point Energies= -1117.938843

Sum of electronic and thermal Free Energies= -1117.997720

The product complex of the intramolecular hydrogen transfer of $(AB\text{-}Pr)^3$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.791157	0.794792	-0.670839
2	6	0	1.992043	0.006543	1.590223
3	6	0	3.241656	-0.509872	1.296316
4	6	0	3.803372	-0.385174	0.014978
5	6	0	3.055106	0.281758	-0.956656
6	1	0	1.248325	1.308967	-1.457967
7	1	0	1.561420	-0.087759	2.581604

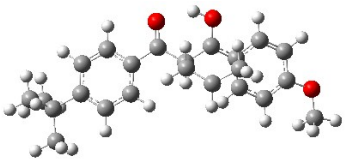
8	1	0	3.794694	-1.022626	2.078200
9	1	0	3.450384	0.408945	-1.957704
10	6	0	5.642067	-0.728005	-1.705723
11	1	0	6.631786	-1.168975	-1.856136
12	1	0	5.716382	0.342040	-1.923797
13	1	0	4.960438	-1.183938	-2.430599
14	6	0	5.135707	-2.498329	-0.029318
15	1	0	4.857110	-2.736742	1.000754
16	1	0	6.118089	-2.940934	-0.224043
17	1	0	4.406798	-2.970168	-0.695030
18	6	0	6.213878	-0.346136	0.686792
19	1	0	5.965104	-0.534825	1.734597
20	1	0	6.263526	0.736919	0.540213
21	1	0	7.207347	-0.765546	0.497171
22	6	0	5.185184	-0.979078	-0.265499
23	6	0	1.244058	0.662603	0.605387
24	6	0	-0.102522	1.192712	0.996814
25	8	0	-0.446870	1.204613	2.158663
26	6	0	-1.038219	1.771692	-0.080973
27	1	0	-0.738346	1.389240	-1.064674
28	6	0	-2.463105	1.355927	0.166051
29	8	0	-3.374008	2.256197	0.620106
30	6	0	-2.888854	0.006326	0.053491
31	6	0	-4.242665	-0.353304	0.289671
32	6	0	-1.998402	-1.030666	-0.302081
33	6	0	-4.663862	-1.657937	0.167011
34	1	0	-4.944739	0.423155	0.570799
35	6	0	-2.424705	-2.347140	-0.428259
36	1	0	-0.948655	-0.814801	-0.481345
37	6	0	-3.762180	-2.670953	-0.194797
38	1	0	-5.697221	-1.934779	0.348074
39	1	0	-1.704554	-3.108899	-0.702471
40	6	0	-3.400976	-4.967915	-0.626934
41	1	0	-2.952656	-4.808813	-1.615666
42	1	0	-3.995826	-5.880937	-0.644222
43	1	0	-2.599402	-5.071194	0.115102
44	8	0	-4.284770	-3.925545	-0.287711
45	6	0	-0.832701	3.296464	-0.070681

46	1	0	0.238089	3.503530	-0.243202
47	1	0	-1.036330	3.671584	0.942974
48	6	0	-1.663516	4.024420	-1.078284
49	1	0	-3.147896	3.137887	0.289341
50	1	0	-1.981488	3.478217	-1.963445
51	6	0	-1.645692	5.514571	-1.119530
52	1	0	-0.709858	5.892287	-1.559794
53	1	0	-1.710775	5.941110	-0.112617
54	1	0	-2.467539	5.915141	-1.717542

Sum of electronic and zero-point Energies= -1117.961945

Sum of electronic and thermal Free Energies= -1118.022475

The reaction complex of the β-bond cleavage of triplet biradical species



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.168198	0.254332	0.599250
2	6	0	3.063211	-1.106473	-1.170313
3	6	0	4.289628	-0.482798	-1.023875
4	6	0	4.491317	0.520782	-0.062480
5	6	0	3.408387	0.870250	0.747042
6	1	0	1.355740	0.554196	1.253543
7	1	0	2.914210	-1.884721	-1.911094

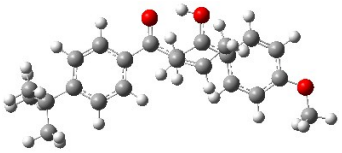
8	1	0	5.111824	-0.781488	-1.667684
9	1	0	3.519620	1.634710	1.506924
10	6	0	5.894398	2.257839	1.148921
11	1	0	6.892717	2.702605	1.194874
12	1	0	5.669830	1.842620	2.136506
13	1	0	5.180670	3.060541	0.938497
14	6	0	6.240419	1.829824	-1.279442
15	1	0	6.285140	1.094767	-2.087733
16	1	0	7.223849	2.304715	-1.202294
17	1	0	5.509133	2.594674	-1.557534
18	6	0	6.907887	0.103529	0.418260
19	1	0	6.968783	-0.670891	-0.351456
20	1	0	6.658167	-0.380863	1.366972
21	1	0	7.898079	0.560472	0.515180
22	6	0	5.866493	1.178271	0.062865
23	6	0	1.980077	-0.739029	-0.362052
24	6	0	0.683516	-1.449016	-0.561563
25	8	0	0.629516	-2.412587	-1.314923
26	6	0	-0.542920	-1.027421	0.236272
27	1	0	-0.455060	0.027354	0.497126
28	6	0	-1.826128	-1.229341	-0.517484
29	8	0	-2.029305	-2.445501	-1.085180
30	6	0	-2.933942	-0.340116	-0.484633
31	6	0	-4.121277	-0.670907	-1.194202
32	6	0	-2.944031	0.869164	0.247168
33	6	0	-5.218549	0.160907	-1.182088
34	1	0	-4.145984	-1.597112	-1.755951
35	6	0	-4.050172	1.709420	0.256616
36	1	0	-2.083592	1.156147	0.842937
37	6	0	-5.197383	1.364099	-0.461471
38	1	0	-6.120964	-0.092127	-1.728740
39	1	0	-4.008222	2.625240	0.834314
40	6	0	-6.332546	3.338680	0.177045
41	1	0	-6.190737	3.189084	1.254828
42	1	0	-7.308655	3.791123	0.002852
43	1	0	-5.549106	4.010820	-0.195046
44	8	0	-6.333172	2.114182	-0.517992
45	6	0	-0.534381	-1.870600	1.563651

46	1	0	0.429689	-1.721479	2.066095
47	1	0	-0.589567	-2.924857	1.262949
48	6	0	-1.673760	-1.525879	2.459951
49	1	0	-1.153947	-2.805301	-1.321305
50	1	0	-1.534816	-0.740801	3.197151
51	6	0	-3.025630	-2.134537	2.297829
52	1	0	-3.330525	-2.687558	3.196894
53	1	0	-3.045237	-2.824354	1.448852
54	1	0	-3.794224	-1.372139	2.115497

Sum of electronic and zero-point Energies= -1117.971667

Sum of electronic and thermal Free Energies= -1118.030751

The transition state of the β-bond cleavage of triplet biradical species



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.217105	-0.638572	-0.177752
2	6	0	3.159515	1.328954	0.823880
3	6	0	4.425861	0.786771	0.684130
4	6	0	4.626616	-0.477358	0.108917

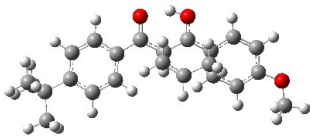
5	6	0	3.494204	-1.173826	-0.319830
6	1	0	1.371729	-1.221032	-0.532428
7	1	0	3.013733	2.308504	1.265906
8	1	0	5.281883	1.360603	1.028575
9	1	0	3.595635	-2.152381	-0.775047
10	6	0	6.063579	-2.413975	-0.688736
11	1	0	7.095229	-2.770495	-0.762700
12	1	0	5.648826	-2.378285	-1.701133
13	1	0	5.497571	-3.148617	-0.107331
14	6	0	6.672185	-1.160193	1.374761
15	1	0	6.730338	-0.190857	1.877662
16	1	0	7.688006	-1.561852	1.297022
17	1	0	6.082195	-1.832496	2.004759
18	6	0	6.891629	-0.074562	-0.877772
19	1	0	6.962798	0.916291	-0.420910
20	1	0	6.457203	0.043121	-1.874990
21	1	0	7.907764	-0.467526	-0.988251
22	6	0	6.045074	-1.034109	-0.024105
23	6	0	2.027374	0.620701	0.398618
24	6	0	0.700334	1.262327	0.585626
25	8	0	0.644168	2.453403	0.990711
26	6	0	-0.508383	0.558659	0.234882
27	1	0	-0.449282	-0.508791	0.073574
28	6	0	-1.825792	1.101116	0.571342
29	8	0	-1.904629	2.417985	0.823406
30	6	0	-3.036991	0.359077	0.528619
31	6	0	-4.266023	1.014652	0.819040
32	6	0	-3.106381	-1.009080	0.177018
33	6	0	-5.465592	0.342158	0.760317
34	1	0	-4.240311	2.063791	1.089790
35	6	0	-4.316444	-1.686256	0.118523
36	1	0	-2.203320	-1.561163	-0.062671
37	6	0	-5.508631	-1.016804	0.411185
38	1	0	-6.402378	0.842254	0.982865
39	1	0	-4.319443	-2.735057	-0.154399
40	6	0	-6.820854	-2.950263	0.039436
41	1	0	-6.432730	-3.130898	-0.970800
42	1	0	-7.877113	-3.215650	0.072369

43	1	0	-6.266821	-3.574643	0.751309
44	8	0	-6.743936	-1.586048	0.383317
45	6	0	-0.353236	1.172017	-1.943196
46	1	0	0.495862	0.523908	-2.138799
47	1	0	-0.127566	2.199602	-1.669133
48	6	0	-1.601755	0.851981	-2.395124
49	1	0	-0.966234	2.727471	0.967728
50	1	0	-1.779802	-0.155092	-2.769394
51	6	0	-2.765236	1.782941	-2.368945
52	1	0	-3.019046	2.101166	-3.388255
53	1	0	-2.548093	2.668278	-1.766001
54	1	0	-3.650399	1.288989	-1.953776

Sum of electronic and zero-point Energies= -1117.943533

Sum of electronic and thermal Free Energies= -1118.002782

The product complex of the β-bond cleavage of triplet biradical species



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.200473	0.527282	0.239079
2	6	0	3.169225	-1.284213	-1.006456
3	6	0	4.423943	-0.725624	-0.830363

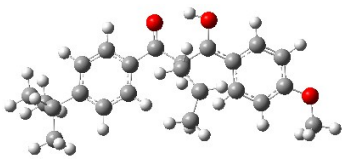
4	6	0	4.604463	0.471835	-0.121068
5	6	0	3.466172	1.080548	0.412587
6	1	0	1.347950	1.013536	0.705290
7	1	0	3.040788	-2.214357	-1.549740
8	1	0	5.286518	-1.232580	-1.254198
9	1	0	3.554257	1.997805	0.983672
10	6	0	6.010128	2.356157	0.842671
11	1	0	7.034427	2.728925	0.935325
12	1	0	5.614694	2.213848	1.853291
13	1	0	5.417163	3.129120	0.343517
14	6	0	6.617174	1.322993	-1.338865
15	1	0	6.685073	0.410888	-1.938285
16	1	0	7.627204	1.732758	-1.233950
17	1	0	6.007824	2.045096	-1.890654
18	6	0	6.889605	0.027965	0.794535
19	1	0	6.961944	-0.917273	0.249580
20	1	0	6.477968	-0.184480	1.785821
21	1	0	7.902782	0.424298	0.919218
22	6	0	6.011941	1.046793	0.048022
23	6	0	2.031769	-0.656333	-0.483200
24	6	0	0.713272	-1.296949	-0.699806
25	8	0	0.649766	-2.508880	-1.055811
26	6	0	-0.491027	-0.545334	-0.528656
27	1	0	-0.425469	0.516331	-0.336018
28	6	0	-1.823054	-1.144523	-0.643108
29	8	0	-1.895174	-2.481209	-0.725864
30	6	0	-3.024392	-0.405193	-0.599140
31	6	0	-4.271760	-1.094157	-0.678094
32	6	0	-3.073546	1.003237	-0.435852
33	6	0	-5.463593	-0.419523	-0.589226
34	1	0	-4.258801	-2.170297	-0.805234
35	6	0	-4.279335	1.681508	-0.346376
36	1	0	-2.159600	1.583743	-0.376446
37	6	0	-5.486290	0.977962	-0.420912
38	1	0	-6.413029	-0.941126	-0.648029
39	1	0	-4.269869	2.757616	-0.221032
40	6	0	-6.782354	2.943849	-0.186336
41	1	0	-6.303852	3.261452	0.748145

42	1	0	-7.841187	3.198062	-0.154608
43	1	0	-6.308079	3.463788	-1.027341
44	8	0	-6.716767	1.543993	-0.346142
45	6	0	-0.371509	-1.390690	2.272613
46	1	0	0.630270	-0.999860	2.426154
47	1	0	-0.455650	-2.342037	1.751516
48	6	0	-1.456899	-0.749595	2.710177
49	1	0	-0.969936	-2.803063	-0.905809
50	1	0	-1.333344	0.200316	3.230617
51	6	0	-2.859550	-1.254346	2.562130
52	1	0	-3.277405	-1.516792	3.540865
53	1	0	-2.891531	-2.138123	1.918550
54	1	0	-3.512842	-0.490716	2.126175

Sum of electronic and zero-point Energies= -1117.949936

Sum of electronic and thermal Free Energies= -1118.011000

The reaction complex of the β-bond cleavage of open shell singlet biradical species



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.080713	-0.409263	0.326719

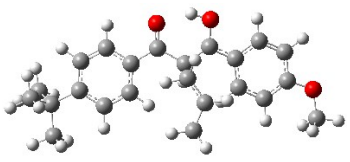
2	6	0	-3.014201	1.606923	-0.593260
3	6	0	-4.238014	0.974769	-0.726176
4	6	0	-4.420233	-0.359887	-0.330801
5	6	0	-3.319016	-1.033987	0.201574
6	1	0	-1.254637	-0.969112	0.755281
7	1	0	-2.881610	2.641083	-0.892919
8	1	0	-5.072639	1.529745	-1.144705
9	1	0	-3.413772	-2.063045	0.527616
10	6	0	-5.806187	-2.466236	-0.012493
11	1	0	-6.806032	-2.887648	-0.150493
12	1	0	-5.556950	-2.542423	1.050643
13	1	0	-5.103097	-3.084075	-0.579930
14	6	0	-6.191456	-0.987615	-1.978963
15	1	0	-6.242414	0.033295	-2.367262
16	1	0	-7.176553	-1.446695	-2.110936
17	1	0	-5.468658	-1.543894	-2.583216
18	6	0	-6.828378	-0.220885	0.326604
19	1	0	-6.896449	0.819073	-0.004087
20	1	0	-6.565320	-0.222013	1.388599
21	1	0	-7.818668	-0.674474	0.216206
22	6	0	-5.794262	-1.011814	-0.492992
23	6	0	-1.913651	0.917810	-0.070051
24	6	0	-0.622086	1.656015	0.056214
25	8	0	-0.599787	2.866289	-0.129626
26	6	0	0.625014	0.903657	0.483204
27	1	0	0.537287	-0.131502	0.148946
28	6	0	1.889441	1.487275	-0.044566
29	8	0	2.028452	2.834387	-0.041682
30	6	0	3.063383	0.722614	-0.287719
31	6	0	4.261304	1.378119	-0.686095
32	6	0	3.121348	-0.680199	-0.133447
33	6	0	5.419262	0.672673	-0.915432
34	1	0	4.244355	2.454818	-0.807090
35	6	0	4.292852	-1.393759	-0.366762
36	1	0	2.241293	-1.235218	0.172702
37	6	0	5.451045	-0.722875	-0.758218
38	1	0	6.332537	1.172969	-1.220352
39	1	0	4.287195	-2.469413	-0.235929

40	6	0	6.714999	-2.719640	-0.864744
41	1	0	6.485478	-3.028727	0.162711
42	1	0	7.738846	-3.004462	-1.106357
43	1	0	6.025546	-3.226236	-1.551726
44	8	0	6.648821	-1.320303	-1.008159
45	6	0	0.611085	0.896586	2.092738
46	1	0	-0.431446	0.774880	2.416267
47	1	0	0.944645	1.895314	2.391355
48	6	0	1.443084	-0.180078	2.664210
49	1	0	1.132871	3.222874	-0.070762
50	1	0	2.514078	-0.029686	2.745086
51	6	0	0.895516	-1.563862	2.765330
52	1	0	0.805157	-2.054796	1.779424
53	1	0	-0.111564	-1.561809	3.200851
54	1	0	1.529810	-2.209844	3.376560

Sum of electronic and zero-point Energies= -1117.972690

Sum of electronic and thermal Free Energies= -1118.029851

The transition state of the β-bond cleavage of open shell singlet biradical species



Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

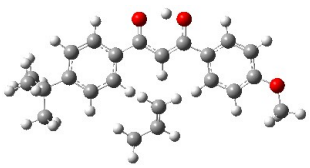
1	6	0	-2.057393	-0.452112	0.171747
2	6	0	-3.046544	1.681242	-0.330015
3	6	0	-4.276171	1.067586	-0.494628
4	6	0	-4.432246	-0.317751	-0.329199
5	6	0	-3.299894	-1.060506	0.012718
6	1	0	-1.207141	-1.067539	0.449214
7	1	0	-2.933112	2.753099	-0.453208
8	1	0	-5.135957	1.677386	-0.756771
9	1	0	-3.373226	-2.131635	0.160258
10	6	0	-5.787668	-2.467056	-0.315434
11	1	0	-6.791452	-2.871811	-0.473551
12	1	0	-5.478556	-2.730282	0.700955
13	1	0	-5.113643	-2.960120	-1.022987
14	6	0	-6.299765	-0.664879	-1.954643
15	1	0	-6.387050	0.407996	-2.146573
16	1	0	-7.285739	-1.114953	-2.109669
17	1	0	-5.609099	-1.085452	-2.691550
18	6	0	-6.795703	-0.334914	0.485577
19	1	0	-6.889260	0.746133	0.350737
20	1	0	-6.465923	-0.520841	1.512136
21	1	0	-7.788755	-0.777569	0.356916
22	6	0	-5.811260	-0.949742	-0.523984
23	6	0	-1.914744	0.924678	-0.002597
24	6	0	-0.617609	1.643231	0.166520
25	8	0	-0.607412	2.872172	0.178156
26	6	0	0.637676	0.853329	0.389299
27	1	0	0.542851	-0.149750	-0.021402
28	6	0	1.865850	1.495929	-0.052734
29	8	0	1.983194	2.837199	0.006674
30	6	0	3.067415	0.763875	-0.301614
31	6	0	4.261897	1.457467	-0.629104
32	6	0	3.141019	-0.638781	-0.189712
33	6	0	5.441420	0.782904	-0.837596
34	1	0	4.226875	2.537529	-0.711433
35	6	0	4.336396	-1.323687	-0.398680
36	1	0	2.258167	-1.217669	0.054372
37	6	0	5.492792	-0.617413	-0.722919
38	1	0	6.356138	1.308421	-1.090344

39	1	0	4.347736	-2.402895	-0.304441
40	6	0	6.800723	-2.584487	-0.840060
41	1	0	6.541698	-2.925985	0.169658
42	1	0	7.838416	-2.839970	-1.052891
43	1	0	6.147228	-3.084972	-1.565244
44	8	0	6.708507	-1.182357	-0.947409
45	6	0	0.663245	0.604043	2.121584
46	1	0	-0.399586	0.517512	2.372794
47	1	0	1.058499	1.557302	2.476788
48	6	0	1.407936	-0.560512	2.508104
49	1	0	1.079629	3.207545	0.095881
50	1	0	2.479181	-0.483066	2.661307
51	6	0	0.795118	-1.917904	2.405509
52	1	0	0.798455	-2.311716	1.371372
53	1	0	-0.253736	-1.906424	2.726083
54	1	0	1.328114	-2.653620	3.013394

Sum of electronic and zero-point Energies= -1117.972089

Sum of electronic and thermal Free Energies= -1118.029065

The product complex of the β-bond cleavage of open shell singlet biradical species



Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.977943	0.184205	-0.330878
2	6	0	2.940966	-1.958682	0.166394
3	6	0	4.206231	-1.396951	0.120246
4	6	0	4.393670	-0.033780	-0.153364
5	6	0	3.253604	0.741035	-0.378732
6	1	0	1.122680	0.828163	-0.510434
7	1	0	2.801786	-3.013646	0.376418
8	1	0	5.068932	-2.032399	0.300514
9	1	0	3.345498	1.798510	-0.600781
10	6	0	5.819110	2.040391	-0.503433
11	1	0	6.850730	2.403789	-0.523041
12	1	0	5.277788	2.610478	0.258276
13	1	0	5.371628	2.252789	-1.479515
14	6	0	6.617109	-0.183945	-1.287471
15	1	0	6.678888	-1.258740	-1.096584
16	1	0	7.637663	0.211223	-1.325372
17	1	0	6.155352	-0.041158	-2.269018
18	6	0	6.487142	0.320572	1.168642
19	1	0	6.547967	-0.741223	1.422494
20	1	0	5.930803	0.826655	1.963273
21	1	0	7.505871	0.721686	1.151399
22	6	0	5.811097	0.539951	-0.195510
23	6	0	1.805696	-1.172744	-0.057225
24	6	0	0.467373	-1.831373	0.010168
25	8	0	0.425574	-3.068588	0.203858
26	6	0	-0.732840	-1.057572	-0.124793
27	1	0	-0.688279	0.010467	-0.257093
28	6	0	-1.952122	-1.686254	-0.010372
29	8	0	-2.032869	-2.984445	0.198355
30	6	0	-3.251276	-0.990536	-0.081175
31	6	0	-4.424113	-1.695627	0.229472
32	6	0	-3.358311	0.354350	-0.441652
33	6	0	-5.656388	-1.072225	0.192700
34	1	0	-4.347676	-2.741382	0.504102
35	6	0	-4.592019	0.994194	-0.482378
36	1	0	-2.471766	0.924114	-0.701145

37	6	0	-5.749622	0.279134	-0.161689
38	1	0	-6.569593	-1.604507	0.434267
39	1	0	-4.639374	2.037595	-0.768728
40	6	0	-7.137325	2.161860	-0.529709
41	1	0	-6.593176	2.816065	0.161657
42	1	0	-8.202513	2.382497	-0.474060
43	1	0	-6.781111	2.340262	-1.551135
44	8	0	-6.997736	0.804010	-0.168081
45	6	0	-0.707524	1.905310	1.508821
46	1	0	0.126451	1.399793	1.990942
47	1	0	-1.702550	1.525097	1.720890
48	6	0	-0.508590	2.931934	0.685172
49	1	0	-1.064110	-3.306362	0.244404
50	1	0	-1.369499	3.409805	0.216939
51	6	0	0.837723	3.503437	0.350444
52	1	0	1.036409	3.445525	-0.726446
53	1	0	1.631567	2.965587	0.876099
54	1	0	0.894678	4.561396	0.626551

Sum of electronic and zero-point Energies= -1118.044302

Sum of electronic and thermal Free Energies= -1118.106187