T. S. Dibble and T. Pham
Peroxy and alkoxy radicals from 2-methyl-3-buten-2-ol

Consisting of
Tables of Electronic and Zero-point energies
Figures of the Structures of all reactants
Tables of Cartesian Coordinates of all reactants and transition states

Table S1. B3LYP/6-31G(d,p) Electronic Energies (E, Hartree) and zero-point energies (ZPE, Hartrees) of **P1**, **P2**, **A1**, **A2**, and **A3.**

Species	E (B3LYP)	ZPE (B3LYP)
P1(2→4,4→3*)	-497.92625	0.16730
P1(4→2,2→3*)	-497.92546	0.16731
P1(2→3*)	-497.91779	0.16564
P1(4→3*)	-497.91942	0.16581
P1(2→4)	-497.92029	0.16618
P1(4→2)	-497.91836	0.16602
P1(none)	-497.91506	0.16520
P2(2→3,3→4*)	-497.92601	0.16638
P2(2→3,3→4*')	-497.92481	0.16615
P2(3→2,2→4*)	-497.92495	0.16682
P2(2→4*)	-497.91903	0.16629
P2(3→4*)	-497.92498	0.16595
P2(2→3)	-497.92345	0.16602
P2(3→2)	-497.92049	0.16565
P2(none)	-497.92074	0.16545
A1(4→2,2→3*)	-422.76485	0.16169
A1(2→4,4→3*)	-422.76434	0.16153
A1(2→3*)	-422.76269	0.16109
A1(4→3*)	-422.76325	0.16103
A1(2→4)	-422.75784	0.15999
A1(4→2)	-422.76265	0.16105
A2(3→2,2→4*)	-422.76799	0.16156
A2(2→3,3→4*)	-422.76233	0.16062
A2(2→4*)	-422.75994	0.16137
A2(3→4*)	-422.76137	0.16039
A2(2→3)	-422.76063	0.15996
A2(3→2)	-422.76124	0.16025
A3(3→4,4→2*)	-422.76766	0.16178
A3(4→3,3→2*)	-422.76438	0.16205
A3(3→2*)	-422.75779	0.16144
A3(4→2*)	-422.76205	0.16123

A3(3→4)	-422.75924	0.16107
A3(4→3)	-422.75831	0.16094

Table S2. B3LYP/6-31G(d,p) Electronic Energies (E, Hartree) and zero-point energies (ZPE, Hartrees) of Transition states for scission and 1,5 H-shift of **A1, A2,** and **A3.**

Reactant	Reaction Type	E	ZPE
A1(4→2,2→3*)	scission 1	-422.75201	0.15906
	scission 2	-422.75449	0.15915
A1(2→4,4→3*)	scission 1	-422.74439	0.15851
	scission 2	-422.76082	0.15976
A1(2→3*)	scission 1	-422.75235	0.15876
	scission 2	-422.7549	0.15925
A1(4→3*)	scission 1	-422.74651	0.15777
	scission 2	-422.75996	0.15951
A1(2→4)	scission 1	-422.74503	0.15846
	scission 2	-422.75662	0.15885
A1(4→2)	scission 1	-422.75160	0.15825
	scission 2	-422.75326	0.15934
A2(3→2,2→4*)	scission	-422.75823	*
	1,5 H-shift	-422.75501	0.15614
A2(2→3,3→4*)	scission	-422.74659	0.15806
A2(2→4*)	scission	-422.75041	0.15855
	1,5 H-shift	-422.74040	0.15622
A2(3→4*)	scission	-422.74331	*
	1,5 H-shift	-422.74200	0.15638
A2(2→3)	scission	-422.74239	0.15783
	1,5 H-shift	-422.73818	0.15589
A2(3→2)	scission	-422.74270	0.15798
	1,5 H-shift	-422.73917	0.15586
A3(3→4,4→2*)	scission	-422.76366	0.16009
A3(4→3,3→2*)	scission	-422.75195	0.15937
A3(3→2*)	scission	-422.74922	0.15905
A3(4→2*)	scission	-422.75648	0.15950
A3(3→4)	scission	-422.75626	0.15971
A3(4→3)	scission	-422.74933	0.15907

* The actual transition state was not found. The number given is an estimate based on scanning energy versus breaking C-C bond length, and the ZPE is not known.

Table S3. B3LYP/6-31G(d,p) and BB1K/6-31+G(d,p) Electronic Energies (E, Hartree) and zero-point energies (ZPE, Hartrees) of Selected conformers of **A1-A3** and their Transition States for H-atom transfer across H-bonds. Values reported in Table S1 are not repeated.

Species	E (B3LYP)	ZPE (B3LYP	E (BB1K)	ZPE (BB1K
A1(4→3*)	S1	S1	-422.57101	0.16481
A1(2→3*)	S1	S1	-422.57296	0.16406
A2(2→4*)	S1	S1	-422.56992	0.16545
A2(3→4*)	S1	S1	-422.57321	0.16427
A3(3→2*)	S1	S1	-422.56841	0.16612
A3(4→2*)	S1	S1	-422.56973	0.16505
[**A1**(4→3*) → **A2**(3→4*)]	-422.73947	0.15596	-422.53733	0.15974
[**A1**(2→3*)→ **A3**(3→2*)]	-422.74094	0.156784	--	--
[**A2**(2→4*)→ **A3**(4→2*)]	-422.75275	0.155853	-422.55244	0.15906

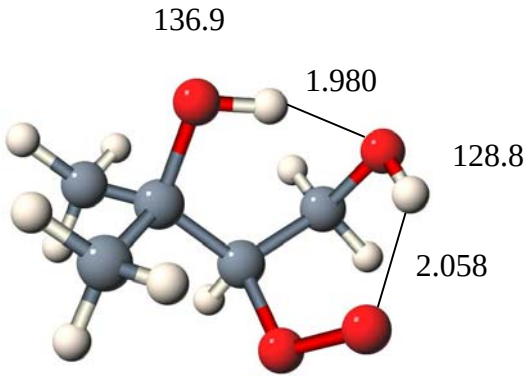
Figure S1. Structure of doubly hydrogen-bonded conformers conformers of peroxy radicals **P1** and **P2.** Thin lines indicate hydrogen bonds. O-H distances (Ångstroms) and OH--O angles (degrees) are listed for hydrogen bonds.

Figure S2. Structure of various conformers of alkoxy radical **A1-A3.** Thin lines indicate hydrogen bonds. O-H distances (Ångstroms) and OH--O angles (degrees) are listed for hydrogen bonds.

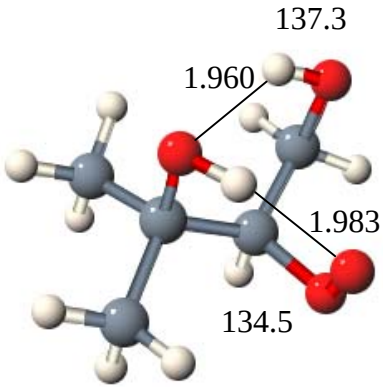
Figure S3. Relative energies of the various conformers of alkoxy radicals **A1-A3**.

Figure S4. Transition state structures for selected β-scission reactions of **A1-A3**. Thin lines indicate hydrogen bonds. Selected interatomic distances (Ångstroms) and angles (degrees) are listed.

Figure S5. Transition state structures for selected 1,5 H-shift reactions of **A2**. Thin lines indicate hydrogen bonds. Selected interatomic distances (Ångstroms) and angles (degrees) are listed.



P1(2→4,4→3*)



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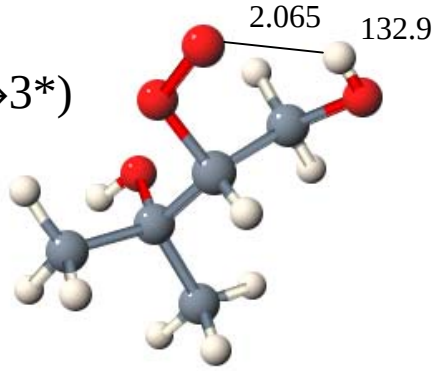
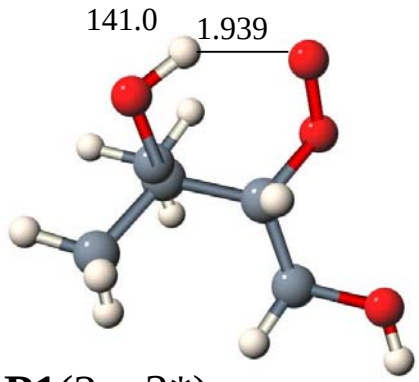
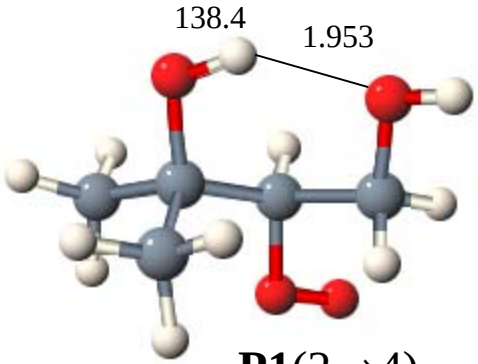


P1(4→3*)



P1(2→3*)



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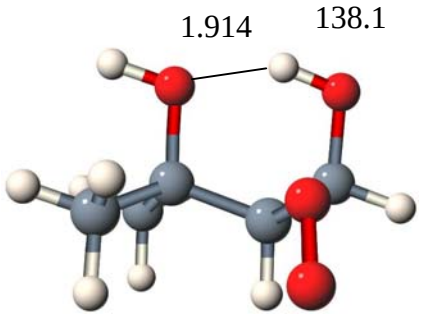

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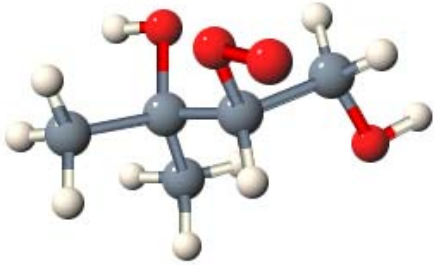
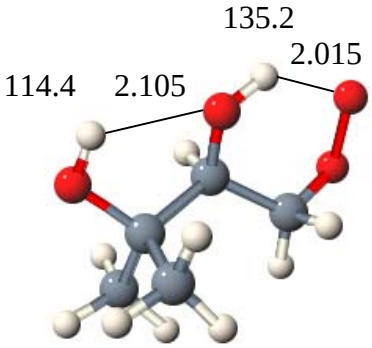
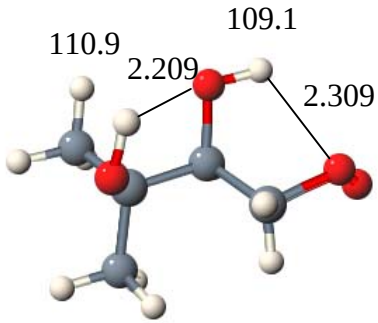


P1(none)

Figure S1



P2(2→3,3→4*)



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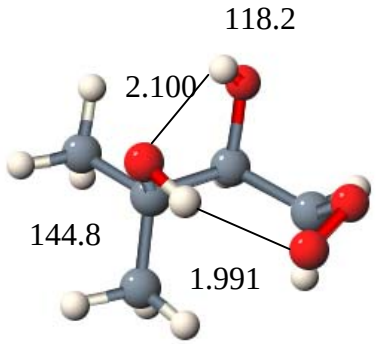
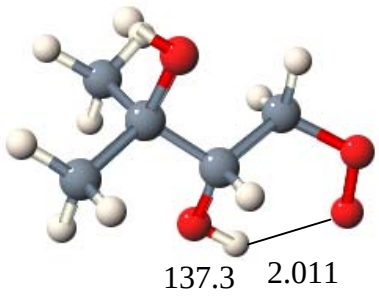


P2(3→2,2→4*)



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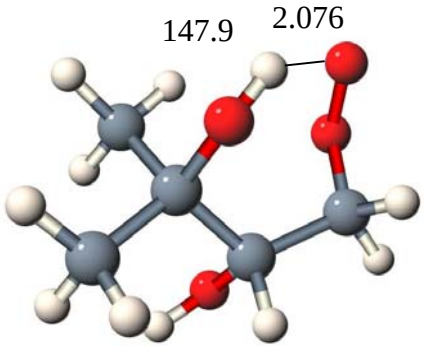

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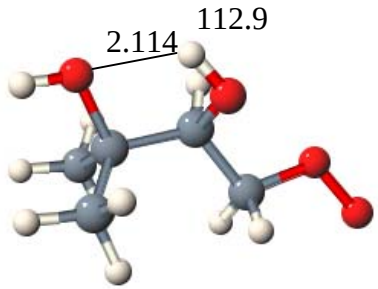

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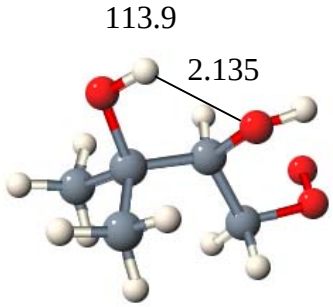
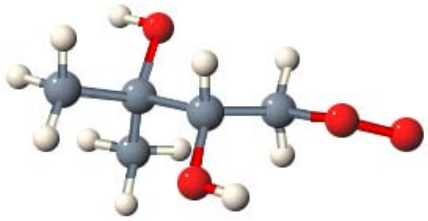


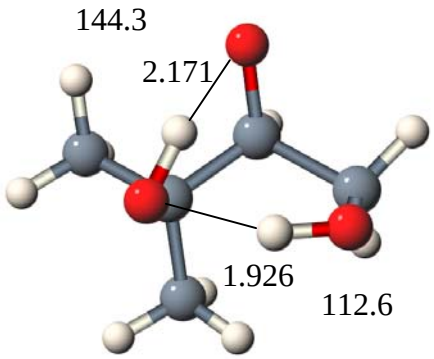
P2(2→3)



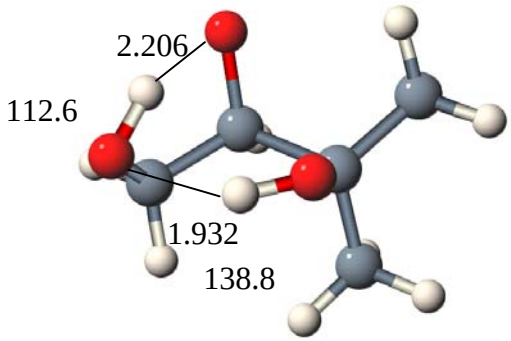
P2(none)

Figure S2

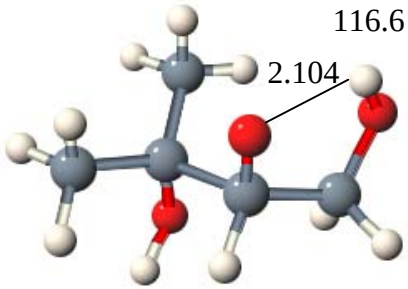
Figure S3



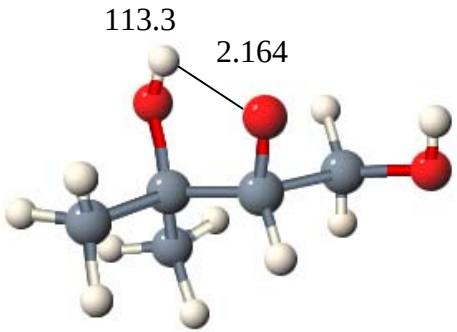
A1(4→2,2→3*)



A1(2 →4,4→3*)



A1(4→3*)



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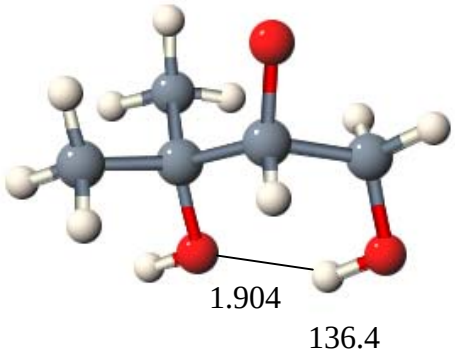

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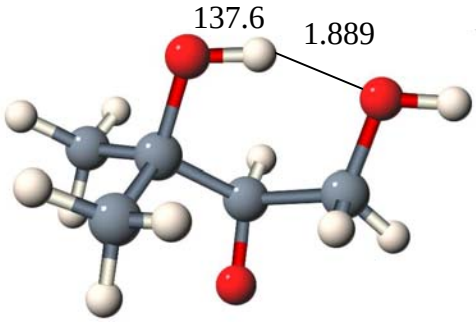
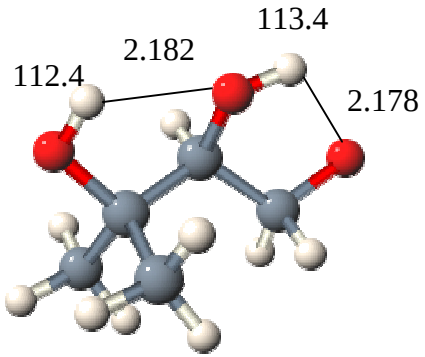
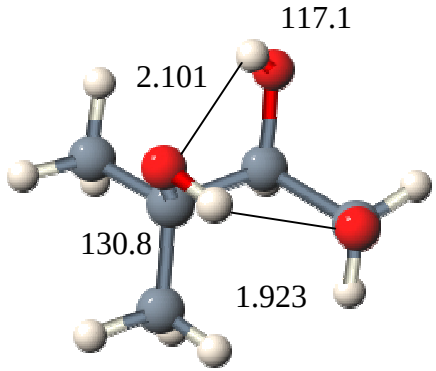


A1(2→4)

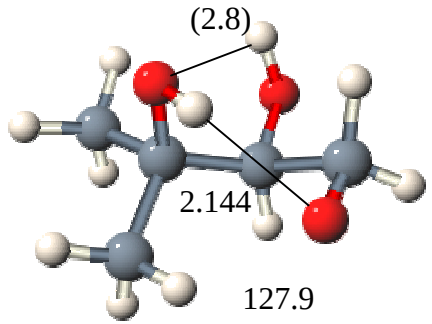
Figure S4



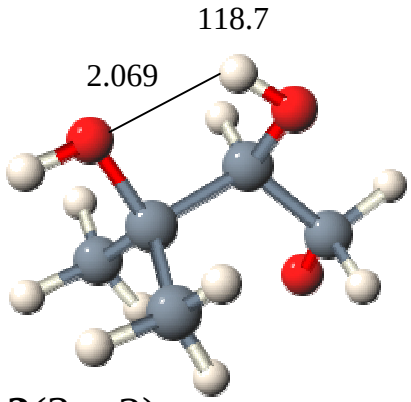
A2(2→3,3→4*)



A2(3→2,2→4*)



A2(2→4*)



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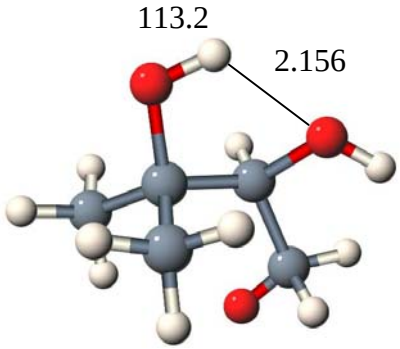

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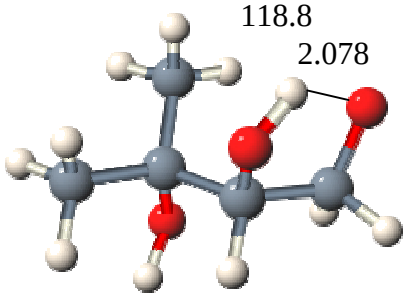
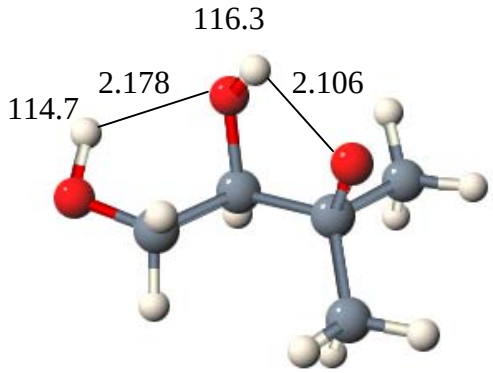
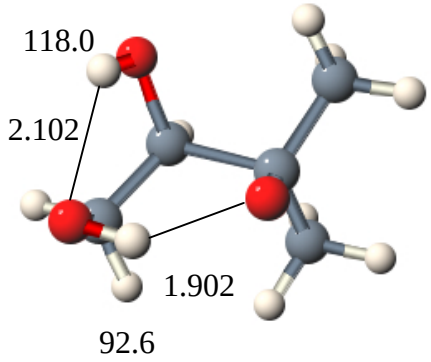


A2(3→4*)

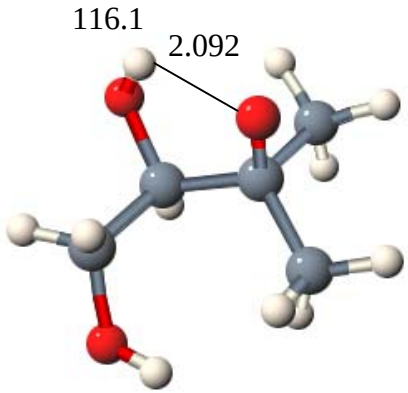
Figure S5



A3(4→3,3→2*)



A3(3→4,4→2*)



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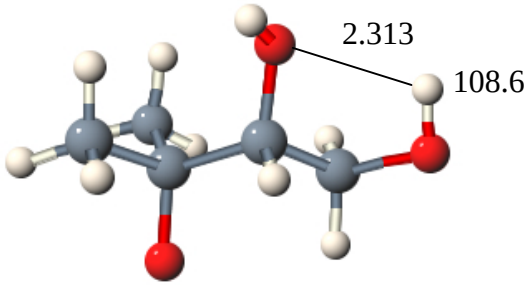

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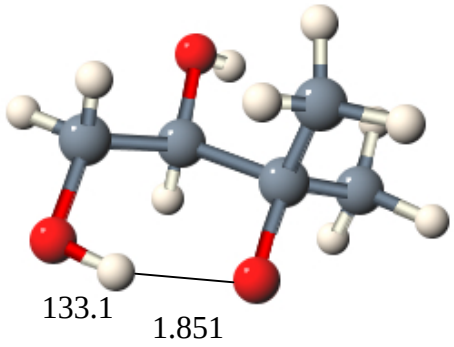

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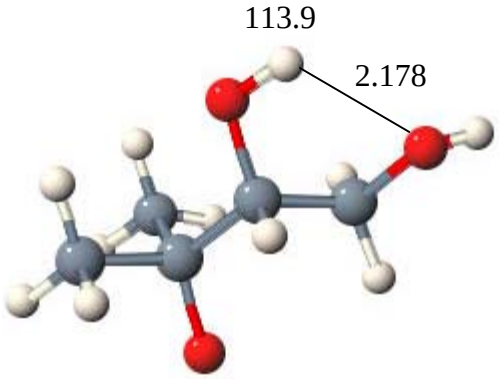

A3(3→4)

Index of Tables of Cartesian Coordinates

Peroxy 1

P1(2→4,4→3*)
P1(4→2,2→3*)
P1(2→3*)
P1(4→3*)
P1(2→4)
P1(4→2)
P1(none)

Peroxy 2

P2(2→3,3→4*)
P2(2→3,3→4*')
P2(3→2,2→4*)
P2(2→4*)
P2(3→4*)
P2(2→3)
P2(3→2)
P2(none)

Alkoxy 1 and related Transition states

A1(4→2,2→3*) scission 1 scission 2
A1(2→4,4→3*) scission 1 scission 2
A1(2→3*) scission 1 scission 2 H-atom transfer
A1(4→3*) scission 1 scission 2 H-atom transfer
A1(2→4)
A1(4→2)

Alkoxy 2

A2(3→2,2→4*) 1,5 H-shift
A2(2→3,3→4*) scission
A2(2→4*) H-atom transfer
A2(3→4*) scission 1,5 H-shift
A2(2→3)
A2(3→2)

Alkoxy 3

A3(3→4,4→2*) scission
A3(4→3,3→2*) scission
A3(3→2*)
A3(4→2*)
A3(3→4)
A3(4→3)

P1(2→4,4→3*)

6	1.346923	0.248981	1.847821
6	0.046852	0.107735	1.050072
6	0.275292	-0.791877	-0.205357
8	-0.317582	1.422754	0.660548
6	-1.055906	-0.519609	1.924120
1	2.127465	0.699483	1.232232
1	1.698084	-0.720835	2.214013
1	1.166248	0.901234	2.706094
1	-0.812226	-1.545723	2.221192
1	-2.020055	-0.528121	1.407130
1	-1.169541	0.081854	2.829719
1	-1.092227	1.330413	0.080035
1	0.638119	-1.772856	0.123289
8	1.421732	-0.284705	-0.969724
6	-0.934018	-0.996749	-1.121282
8	1.090553	0.621775	-1.878921
1	-0.963312	0.718003	-1.963158
1	-0.599965	-1.528963	-2.022719
8	-1.618622	0.204368	-1.460636
1	-1.656100	-1.638913	-0.610204

P1(4→2,2→3*)

6	-0.651666	-2.065115	-0.464735
6	-0.706301	-0.529053	-0.459318
6	0.720492	0.081146	-0.533237
8	-1.382027	-0.068562	0.724752
6	-1.548818	-0.027722	-1.637439
1	-0.094975	-2.449571	0.392532
1	-0.176664	-2.442244	-1.376416
1	-1.670834	-2.457089	-0.417002
1	-1.105261	-0.314796	-2.595341
1	-1.665843	1.058309	-1.614019
1	-2.545353	-0.471435	-1.570517
1	-0.801714	-0.327588	1.463164
1	1.185613	-0.208147	-1.482483
8	1.639780	-0.529577	0.437105
6	0.813052	1.611198	-0.398741
8	1.153154	-0.589797	1.670470
1	-0.598876	1.719434	0.899156
1	1.871444	1.890997	-0.426930
8	0.276482	2.129865	0.790972
1	0.342798	2.043970	-1.297711

P1(2→3*)

6	-0.827924	-2.126025	-0.038660
6	-0.889840	-0.610700	0.196772

6	0.529939	0.009779	0.065970
8	-1.321531	-0.470115	1.548089
6	-1.902296	0.054514	-0.750262
1	-0.027243	-2.582633	0.551154
1	-0.685969	-2.379960	-1.092367
1	-1.775304	-2.556926	0.295203
1	-1.628449	-0.072009	-1.803431
1	-1.985241	1.124481	-0.544186
1	-2.883578	-0.400337	-0.593107
1	-1.081515	0.425626	1.839502
1	1.141404	-0.337121	0.904142
8	0.461116	1.479566	0.177620
6	1.271813	-0.214873	-1.242260
8	0.092954	1.897240	1.377519
1	3.058496	0.211947	-1.897890
1	1.209474	-1.277664	-1.511423
8	2.615614	0.193753	-1.040516
1	0.782551	0.364866	-2.038642

P1(4→3*)

6	-1.118534	-2.034447	-0.137214
6	-1.096525	-0.498560	-0.209331
6	0.344818	0.046787	-0.236355
8	-1.690336	0.062501	0.967609
6	-1.851426	-0.020948	-1.462595
1	-0.651906	-2.387297	0.783141
1	-0.597205	-2.483599	-0.988479
1	-2.156278	-2.386798	-0.161672
1	-1.394521	-0.404745	-2.380085
1	-1.887669	1.069121	-1.519884
1	-2.882664	-0.389053	-1.427701
1	-2.581834	-0.301280	1.051602
1	0.815587	-0.180179	-1.198199
8	1.101483	-0.714855	0.777779
6	0.494282	1.544623	0.062092
8	2.389416	-0.414802	0.778132
1	2.414461	1.499013	0.003666
1	-0.289995	2.097918	-0.460545
8	1.729140	2.060408	-0.391038
1	0.338705	1.696148	1.138720

P1(2→4)

6	-0.985726	-1.719363	0.213533
6	-1.026797	-0.200416	-0.013562
6	0.390841	0.411876	-0.176465
8	-1.646754	0.456564	1.090751

6	-1.885879	0.143946	-1.233027
1	-0.487981	-1.964852	1.156873
1	-0.463962	-2.235181	-0.599296
1	-2.008217	-2.102058	0.269119
1	-1.515739	-0.345474	-2.136675
1	-1.899222	1.225431	-1.396632
1	-2.912256	-0.182782	-1.045378
1	-1.037144	0.386411	1.843517
1	0.293371	1.497714	-0.254021
8	0.948526	-0.067751	-1.445156
6	1.417715	0.043913	0.897999
8	1.947132	0.697817	-1.861089
1	1.503160	0.122218	2.857808
1	1.628166	-1.032590	0.843305
8	0.887683	0.409065	2.172022
1	2.346194	0.585878	0.678285

P1(4→2)

6	-0.792193	-1.939051	-0.273622
6	-0.816684	-0.409531	-0.382887
6	0.612513	0.186615	-0.323281
8	-1.530835	0.141738	0.742530
6	-1.503629	0.026390	-1.687858
1	-0.385038	-2.250358	0.689176
1	-0.185008	-2.386219	-1.065587
1	-1.811230	-2.332209	-0.367838
1	-0.966730	-0.344451	-2.566487
1	-1.579871	1.114078	-1.757078
1	-2.518630	-0.384538	-1.724091
1	-2.418764	-0.238986	0.757308
1	1.134243	-0.085343	-1.245041
8	1.375594	-0.438811	0.761192
6	0.707703	1.704048	-0.104215
8	2.168955	-1.399251	0.311250
1	-0.607665	1.723582	1.296923
1	1.763217	1.985928	-0.178515
8	0.254246	2.144948	1.151742
1	0.185540	2.198687	-0.941315

P1(none)

6	-0.724727	-2.139069	-0.009670
6	-0.867039	-0.609178	-0.072966
6	0.519934	0.064181	-0.140367
8	-1.464986	-0.122381	1.136508
6	-1.719632	-0.202789	-1.285720
1	-0.185109	-2.442964	0.888379

1	-0.194124	-2.526477	-0.885568
1	-1.718818	-2.600746	0.004636
1	-1.266913	-0.539396	-2.223711
1	-1.839001	0.879352	-1.334413
1	-2.706731	-0.673261	-1.205271
1	-2.325193	-0.552498	1.230415
1	1.018331	-0.190590	-1.079871
8	1.326272	-0.526860	0.939045
6	0.554517	1.581409	0.055048
8	2.619175	-0.339600	0.734298
1	0.064867	3.140858	-1.006364
1	-0.104045	1.853173	0.888043
8	0.155732	2.193739	-1.168096
1	1.588879	1.846045	0.311733

P2(2→3,3→4*)

1	-0.255677	-1.197470	-2.138143
6	-0.394163	-0.113702	-2.175709
1	0.569999	0.349522	-2.415835
6	-0.972127	0.399254	-0.846632
1	-1.093241	0.119987	-2.982738
6	-0.123454	-0.067087	0.368299
8	-2.280476	-0.137200	-0.652606
6	-1.147777	1.918615	-0.862240
1	-0.213169	2.440946	-1.087505
1	-1.532227	2.274471	0.098073
1	-1.875647	2.182552	-1.634070
8	-0.259301	-1.482320	0.425753
1	-0.559682	0.397518	1.266498
6	1.349556	0.327321	0.300244
8	1.996412	0.202426	1.610317
1	1.496311	1.382171	0.060424
1	1.900288	-0.305551	-0.400057
1	-2.152214	-1.062986	-0.393306
1	0.334218	-1.793149	1.128411
8	1.931969	-1.029709	2.090844

P2(2→3,3→4’)

1	-0.295462	-0.971686	-2.301725
6	-0.207485	0.117321	-2.271450
1	0.830587	0.396380	-2.478123
6	-0.675717	0.677461	-0.926810
1	-0.835587	0.519785	-3.070618
6	0.237257	0.233132	0.244401
8	-1.981383	0.138030	-0.699838
6	-0.738235	2.212832	-0.975272

1	0.239180	2.643528	-1.218396
1	-1.056838	2.617421	-0.011614
1	-1.454868	2.520350	-1.741462
8	-0.402200	0.705163	1.430322
1	1.233413	0.687187	0.134715
6	0.404349	-1.282819	0.322018
8	1.100018	-1.629927	1.561022
1	0.987712	-1.690418	-0.503988
1	-0.567231	-1.774155	0.400732
1	-2.214744	0.394036	0.206037
1	0.067643	0.336851	2.191031
8	2.401713	-1.391621	1.463005

P2(3→2,2→4*)

1	0.240918	-0.880457	-1.986166
6	0.436842	0.194767	-1.973217
1	1.510042	0.352975	-2.128262
6	-0.033978	0.836154	-0.663843
1	-0.095450	0.647581	-2.814448
6	0.769382	0.353922	0.585359
8	-1.425329	0.559141	-0.427853
6	0.061541	2.363259	-0.747732
1	1.081780	2.676886	-0.989808
1	-0.223646	2.815818	0.204045
1	-0.611866	2.727795	-1.527504
8	0.143017	0.823826	1.761885
1	1.767513	0.813173	0.535601
6	1.056190	-1.152011	0.720864
8	-0.123318	-1.960958	1.031704
1	1.683646	-1.308075	1.601075
1	1.530916	-1.584563	-0.162641
1	-1.553138	-0.396982	-0.538641
1	-0.809240	0.767618	1.568450
8	-0.877036	-2.198048	-0.027022

P2(2→4*)

1	-2.164102	0.002962	-2.024739
6	-1.100704	-0.164268	-2.220085
1	-0.959115	-1.208295	-2.523165
6	-0.269133	0.184539	-0.979336
1	-0.803530	0.471113	-3.058073
6	-0.710438	-0.746258	0.201187
8	-0.627751	1.529701	-0.658345
6	1.228553	0.064058	-1.304070
1	1.498466	-0.965191	-1.552471
1	1.856514	0.376160	-0.467867

1	1.457914	0.703283	-2.161474
8	-0.128657	-2.043240	0.149391
1	-1.811654	-0.816635	0.147702
6	-0.477616	-0.206615	1.610031
8	0.914201	0.104992	1.931426
1	-0.741217	-0.982651	2.332200
1	-1.059604	0.698918	1.780178
1	-0.008192	1.835555	0.025025
1	-0.383680	-2.453554	-0.686792
8	1.228986	1.352247	1.620417

P2(3→4*)

1	-0.173119	-1.577822	-2.393268
6	-0.181598	-0.485912	-2.460221
1	0.828646	-0.141449	-2.691518
6	-0.678412	0.121644	-1.142975
1	-0.843091	-0.196452	-3.285381
6	0.257633	-0.324589	0.007349
8	-1.952399	-0.440009	-0.788061
6	-0.775222	1.649478	-1.246664
1	0.216445	2.090372	-1.371650
1	-1.240719	2.076692	-0.353551
1	-1.389221	1.932108	-2.109383
8	1.553995	0.171854	-0.268483
1	0.244593	-1.426850	0.018389
6	-0.242649	0.140090	1.375975
8	0.413194	-0.605133	2.450971
1	-1.300951	-0.083907	1.510409
1	-0.038130	1.200537	1.543241
1	-2.568087	-0.242909	-1.506162
1	2.075763	0.038636	0.539773
8	1.723880	-0.410864	2.467862

P2(2→3)

1	-0.148392	-1.371481	-2.184187
6	-0.246421	-0.284158	-2.245559
1	0.744570	0.140415	-2.441664
6	-0.874452	0.275982	-0.958525
1	-0.893851	-0.041233	-3.091979
6	-0.122819	-0.204029	0.309187
8	-2.217237	-0.195562	-0.835917
6	-0.974302	1.801863	-1.004478
1	-0.002772	2.272828	-1.180750
1	-1.393743	2.191162	-0.072249
1	-1.643140	2.088349	-1.820465
8	-0.287278	-1.623550	0.353388

1	-0.610884	0.261238	1.177192
6	1.358557	0.150064	0.363839
8	1.925165	-0.332516	1.625020
1	1.539841	1.225155	0.313696
1	1.931028	-0.381391	-0.399060
1	-2.145798	-1.126127	-0.572703
1	0.017760	-1.934599	1.215895
8	1.549599	0.431297	2.641195

P2(3→2)

1	-1.455624	0.469467	-1.972861
6	-0.383983	0.660722	-2.062008
1	0.107823	-0.255650	-2.403516
6	0.177957	1.136962	-0.718142
1	-0.221685	1.421362	-2.834973
6	-0.234522	0.193877	0.447396
8	-0.465925	2.369862	-0.331577
6	1.692639	1.361126	-0.774063
1	2.236419	0.454055	-1.054944
1	2.064855	1.707805	0.194121
1	1.929711	2.127079	-1.520539
8	-1.641123	0.190223	0.603705
1	0.255913	0.580071	1.356464
6	0.201124	-1.247240	0.254727
8	0.117019	-1.904176	1.555418
1	1.236105	-1.335557	-0.083697
1	-0.466037	-1.777251	-0.428694
1	-0.453532	2.968194	-1.089985
1	-1.897212	1.125677	0.602049
8	0.483027	-3.170650	1.466093

P2(none)

1	-0.148392	-1.371481	-2.184187
6	-0.246421	-0.284158	-2.245559
1	0.744570	0.140415	-2.441664
6	-0.874452	0.275982	-0.958525
1	-0.893851	-0.041233	-3.091979
6	-0.122819	-0.204029	0.309187
8	-2.217237	-0.195562	-0.835917
6	-0.974302	1.801863	-1.004478
1	-0.002772	2.272828	-1.180750
1	-1.393743	2.191162	-0.072249
1	-1.643140	2.088349	-1.820465
8	-0.287278	-1.623550	0.353388
1	-0.610884	0.261238	1.177192
6	1.358557	0.150064	0.363839

8	1.925165	-0.332516	1.625020
1	1.539841	1.225155	0.313696
1	1.931028	-0.381391	-0.399060
1	-2.145798	-1.126127	-0.572703
1	0.017760	-1.934599	1.215895
8	1.549599	0.431297	2.641195

A1(4→2, 2→3*)

1	-2.206683	-0.142747	-0.076383
6	-1.621018	-0.466312	-0.940809
1	-1.675529	-1.556505	-1.015178
6	-0.172731	0.005123	-0.836453
1	-2.083177	-0.040507	-1.836324
6	0.639148	-0.670764	0.326913
8	-0.223238	1.412847	-0.550981
6	0.585539	-0.240336	-2.149475
1	0.621928	-1.309584	-2.383958
1	1.615284	0.122572	-2.069745
1	0.092964	0.280649	-2.974881
8	1.797320	-0.007847	0.537167
1	0.794748	-1.747840	0.129602
6	-0.156607	-0.648912	1.711689
8	-0.604123	0.614994	2.081199
1	0.513608	-1.033862	2.487143
1	-0.976180	-1.374705	1.575009
1	-0.791489	1.115023	1.264994
1	0.688872	1.654748	-0.310552

A1(4→2,2→3*) TS for scission 1

1	0.027638	-2.148082	-0.443504
6	-0.902804	-1.601769	-0.614028
1	-1.076526	-1.536848	-1.693329
6	-0.873306	-0.208885	0.007733
1	-1.712911	-2.192255	-0.177103
6	0.025340	0.835916	-0.709682
8	-0.378113	-0.327880	1.353801
6	-2.293477	0.391472	0.039873
1	-2.710207	0.480494	-0.969219
1	-2.269602	1.387702	0.489116
1	-2.949091	-0.252648	0.632729
8	0.304038	1.869390	-0.080580
1	0.016314	0.817208	-1.818569
6	1.985230	-0.234434	-0.663148
8	2.250482	-0.396044	0.644498
1	2.654066	0.466440	-1.154598

1	1.652468	-1.096462	-1.242807
1	1.454580	-0.773500	1.079177
1	-0.143878	0.590418	1.591858

A1(4→2,2→3*) TS for scission 2

1	-0.283899	-2.197124	-0.496023
6	-1.143072	-1.544007	-0.660170
1	-1.272604	-1.379388	-1.733128
6	-0.993921	-0.234493	0.063316
1	-2.036986	-2.065098	-0.291013
6	0.574478	0.778747	-0.705737
8	-0.567129	-0.427708	1.363225
6	-2.131183	0.752103	-0.080769
1	-2.362281	0.936769	-1.132978
1	-1.878369	1.704587	0.388047
1	-3.026873	0.339004	0.401060
8	0.551600	1.758946	0.092813
1	0.158022	0.894535	-1.732607
6	1.750471	-0.217558	-0.670057
8	2.163251	-0.609265	0.615882
1	2.598459	0.312667	-1.125302
1	1.526650	-1.074006	-1.327904
1	1.372165	-0.907123	1.090431
1	-0.316698	0.450637	1.704551

A1(2→4,4→3*)

1	1.905599	0.701937	1.545397
6	1.023092	0.205399	1.949090
1	1.304676	-0.791891	2.298743
6	-0.074693	0.131067	0.890321
1	0.652723	0.780998	2.802873
6	0.483357	-0.774339	-0.392758
8	-0.355141	1.437768	0.479810
6	-1.333919	-0.564567	1.432079
1	-1.143080	-1.607097	1.703997
1	-2.159568	-0.532898	0.716708
1	-1.656508	-0.025654	2.328023
1	0.590659	-1.785413	0.043848
8	1.641473	-0.231681	-0.780166
6	-0.533785	-0.756589	-1.560428
8	-0.616007	0.555939	-2.103386
1	-1.538763	-1.049688	-1.248590
1	-0.194776	-1.475622	-2.320013
1	-0.819789	1.399221	-0.377033

1	0.311928	0.844075	-2.173848

A1(2→4,4→3*) TS for scission 1

1	2.017892	1.632559	0.585814
6	2.217084	0.683025	0.084881
1	2.600086	0.881283	-0.921145
6	0.926605	-0.153780	0.043411
1	2.979297	0.136731	0.648184
6	-0.121942	0.729879	-0.689567
8	0.567780	-0.367233	1.400737
6	1.178227	-1.486956	-0.676201
1	1.402886	-1.341314	-1.738899
1	0.316991	-2.157915	-0.597205
1	2.030230	-1.993824	-0.214929
1	-0.036506	0.688553	-1.799385
8	-0.613987	1.736157	-0.135138
6	-1.915782	-0.394838	-0.664015
8	-2.230576	-0.465827	0.658971
1	-1.728186	-1.372998	-1.095770
1	-2.470700	0.321938	-1.265346
1	-0.330694	-0.729733	1.413941
1	-2.272185	0.445963	0.997128

A1(2→4,4→3*) TS for scission 2

1	1.599302	1.812492	0.690071
6	2.025611	0.962295	0.156935
1	2.323091	1.276921	-0.846497
6	1.031396	-0.169049	0.109277
1	2.923961	0.625353	0.691011
6	-0.619433	0.643596	-0.793829
8	0.610130	-0.491932	1.364277
6	1.391207	-1.335144	-0.791038
1	1.527577	-1.014390	-1.827504
1	0.645166	-2.132363	-0.759488
1	2.340835	-1.762554	-0.442872
1	-0.147241	0.722364	-1.792964
8	-0.838329	1.683543	-0.110140
6	-1.669625	-0.472125	-0.639615
8	-2.025611	-0.576662	0.734532
1	-1.333062	-1.453141	-0.982150
1	-2.543001	-0.191737	-1.250906
1	-0.265429	-0.932324	1.321247
1	-1.995648	0.352349	1.040321

A1(2→3*)

1	0.723649	2.174067	-1.287378

6	0.619842	2.195318	-0.197646
1	1.623978	2.228803	0.239283
6	-0.170151	0.965188	0.285777
1	0.086348	3.107358	0.083499
6	0.537578	-0.311350	-0.268447
8	-1.488214	0.988665	-0.255500
6	-0.307827	0.977606	1.807552
1	0.662268	0.827670	2.293383
1	-1.000419	0.204624	2.149234
1	-0.704296	1.943096	2.134286
1	1.601097	-0.374800	0.026246
8	0.375120	-0.423680	-1.605300
6	-0.100878	-1.665902	0.309475
8	0.556515	-2.791765	-0.185748
1	-1.169808	-1.628108	0.070886
1	0.039391	-1.653806	1.391645
1	0.494740	-2.760256	-1.151029
1	-1.375700	0.780429	-1.197944

A1(2→3*) TS for scission 1

1	-2.029304	-1.799087	-0.332582
6	-2.175656	-0.751202	-0.609626
1	-2.180402	-0.682915	-1.703071
6	-1.061704	0.119030	0.016703
1	-3.147979	-0.419351	-0.234717
6	0.271210	-0.460548	-0.489523
8	-1.086609	-0.004470	1.434121
6	-1.264517	1.589726	-0.340229
1	-1.117100	1.752874	-1.413209
1	-0.574382	2.230210	0.213891
1	-2.282235	1.900952	-0.088054
1	0.530828	-0.230335	-1.541374
8	0.708251	-1.509349	0.053184
6	1.811379	0.791188	0.200484
8	2.877235	0.108742	-0.260413
1	1.504550	0.652872	1.236373
1	1.743144	1.793846	-0.212496
1	2.737534	-0.826772	-0.017642
1	-0.659946	-0.860837	1.610902

A1(2→3*) TS for scission 2

1	-1.687149	-1.887842	-0.433689
6	-2.032443	-0.878064	-0.664317
1	-1.984278	-0.732443	-1.746525
6	-1.196015	0.153013	0.062693
1	-3.078627	-0.774223	-0.349058

6	0.660223	-0.421821	-0.480851
8	-1.131423	0.007248	1.420117
6	-1.404029	1.591619	-0.324810
1	-1.200990	1.743979	-1.388063
1	-0.773218	2.256407	0.267822
1	-2.450699	1.871047	-0.141215
1	0.484452	-0.384581	-1.575960
8	0.722688	-1.551888	0.093701
6	1.569484	0.687974	0.061481
8	2.923092	0.307255	-0.144630
1	1.344051	0.844685	1.126072
1	1.427501	1.628554	-0.477676
1	3.010220	-0.574363	0.247118
1	-0.789437	-0.888461	1.592493

A1(2→3*)TS for H-atom transfer

1	-1.591949	-1.792393	-0.771046
6	-2.082478	-0.820242	-0.851024
1	-2.027769	-0.455855	-1.880038
6	-1.487703	0.153990	0.132228
1	-3.147186	-0.963252	-0.607229
6	0.967794	-0.578762	-0.531274
8	-1.072208	-0.269333	1.277328
6	-1.770962	1.619571	-0.021734
1	-1.650544	1.949527	-1.058025
1	-1.125303	2.205713	0.635144
1	-2.813514	1.829078	0.262363
1	0.985602	-0.894099	-1.581819
8	0.738189	-1.471770	0.368919
6	1.652490	0.714088	-0.169349
8	3.072028	0.517939	-0.121502
1	1.266509	1.075350	0.794121
1	1.483660	1.478881	-0.932529
1	3.230293	-0.173415	0.537046
1	-0.188717	-1.006088	1.050968

A1(4→3*)

1	0.070398	1.719378	-0.973482
6	0.028613	1.701504	0.116263
1	1.045753	1.808368	0.499158
6	-0.585375	0.405074	0.623671
1	-0.579663	2.540781	0.467512
6	0.255158	-0.914268	0.027724
8	-1.888635	0.324688	0.102915
6	-0.581657	0.302027	2.147582
1	0.439679	0.319986	2.531419

1	-1.048473	-0.632235	2.482673
1	-1.144567	1.139718	2.571412
1	-0.318483	-1.752850	0.473522
8	1.498146	-0.818689	0.496972
6	0.205247	-0.967577	-1.517902
8	1.197464	-0.140656	-2.082918
1	-0.773003	-0.644629	-1.883588
1	0.348618	-2.022152	-1.809661
1	1.945471	-0.198957	-1.463778
1	-2.373447	-0.360708	0.585039

A1(4→3*) TS for scission 1

1	-0.250186	-1.274919	1.448340
6	0.613580	-0.608485	1.443535
1	0.372673	0.271210	2.044775
6	0.952031	-0.175275	0.021315
1	1.463181	-1.130482	1.891903
6	-0.116269	0.770221	-0.577063
8	1.053029	-1.364127	-0.772972
6	2.282120	0.600605	-0.016301
1	2.218167	1.502443	0.598238
1	2.531676	0.911154	-1.039203
1	3.090946	-0.034107	0.357962
1	-0.059410	0.806121	-1.692107
8	-0.594378	1.726426	0.063452
6	-1.881723	-0.436767	-0.701377
8	-2.409501	-0.381849	0.539024
1	-1.539625	-1.426473	-0.984539
1	-2.327761	0.199915	-1.465251
1	-2.459679	0.555412	0.796504
1	1.468373	-1.125671	-1.613315

A1(4→3*) TS for scission 2

1	-0.144846	-1.436540	1.327815
6	0.714143	-0.766748	1.393988
1	0.458663	0.055441	2.064052
6	1.089342	-0.224412	0.043589
1	1.565748	-1.319347	1.812669
6	-0.601573	0.739467	-0.601224
8	1.286772	-1.239858	-0.858935
6	2.102804	0.892354	-0.001764
1	1.733582	1.753238	0.557518
1	2.299518	1.215722	-1.031168
1	3.052391	0.557773	0.436548
1	-0.103797	1.028654	-1.550621
8	-0.803612	1.615152	0.286720

6	-1.648188	-0.371516	-0.746362
8	-2.325094	-0.565440	0.472536
1	-1.195892	-1.313983	-1.070728
1	-2.337718	-0.044121	-1.547683
1	-2.232635	0.292416	0.927609
1	1.701296	-0.882958	-1.657936

A1(4→3*) TS for H-atom transfer

1	-0.125019	-1.138271	1.647473
6	0.686696	-0.419775	1.510043
1	0.420243	0.497246	2.038601
6	0.943110	-0.126586	0.036994
1	1.594181	-0.839916	1.952636
6	-0.407206	0.379219	-0.684654
8	1.343918	-1.343372	-0.571534
6	2.005499	0.960123	-0.151142
1	1.664224	1.907260	0.271631
1	2.212936	1.124508	-1.215973
1	2.936828	0.658766	0.338207
1	-0.117359	0.585344	-1.728539
8	-0.919739	1.483990	-0.074035
6	-1.542979	-0.697445	-0.546931
8	-2.339089	-0.228172	0.470993
1	-1.198498	-1.723678	-0.383577
1	-2.091563	-0.685078	-1.511645
1	-1.825162	0.879842	0.433026
1	1.737748	-1.138806	-1.431092

A1(2→4)

1	-0.641962	1.974316	0.101279
6	-0.256769	1.452700	0.981864
1	0.769421	1.781088	1.166468
6	-0.314216	-0.065780	0.798525
1	-0.882492	1.731570	1.835386
6	0.749130	-0.517422	-0.411684
8	-1.585158	-0.504225	0.414390
6	0.061626	-0.819640	2.067350
1	1.044450	-0.512827	2.427934
1	0.075777	-1.896774	1.881393
1	-0.691569	-0.615970	2.834764
1	0.472894	-1.579658	-0.542789
8	1.977854	-0.325925	0.065583
6	0.510610	0.286213	-1.705123
8	-0.873810	0.241540	-2.070433
1	1.130794	-0.155104	-2.497371
1	0.853561	1.315052	-1.539764

1	-1.001945	0.751608	-2.879221
1	-1.782303	-0.100844	-0.449990

A1(4→2)

1	0.670330	1.882655	-0.930840
6	0.624849	1.785494	0.157330
1	1.643165	1.687968	0.539749
6	-0.213309	0.575055	0.573278
1	0.191127	2.708313	0.559561
6	0.451138	-0.770201	0.142897
8	-1.496991	0.596469	-0.093576
6	-0.429151	0.547933	2.090197
1	0.529535	0.459287	2.609996
1	-1.058367	-0.301681	2.371323
1	-0.918132	1.468003	2.431847
1	-0.171540	-1.618474	0.485956
8	1.733730	-0.873942	0.521619
6	0.444557	-0.969663	-1.462123
8	-0.833014	-1.260109	-1.929938
1	1.095464	-1.817502	-1.680782
1	0.875035	-0.061210	-1.902090
1	-1.405357	-0.534934	-1.622567
1	-1.949573	1.416527	0.143538

A2(3→2,2→4*)

1	0.338523	1.969535	-0.953982
6	0.454394	1.868581	0.128326
1	1.515316	1.975142	0.378761
6	-0.100736	0.528026	0.616954
1	-0.092178	2.685433	0.607610
6	0.667232	-0.698727	0.048954
8	-1.467448	0.363881	0.217288
6	-0.097120	0.460651	2.149731
1	0.913379	0.611702	2.540932
1	-0.462398	-0.508955	2.493624
1	-0.747218	1.243454	2.548550
8	0.010743	-1.879045	0.362290
1	1.692547	-0.767845	0.430002
6	0.855414	-0.567848	-1.570396
8	-0.329049	-0.260083	-2.110965
1	1.242559	-1.558680	-1.859356
1	1.630065	0.210148	-1.698569
1	-1.481862	0.466517	-0.753699
1	-0.937795	-1.668570	0.275822

A2(3→2,2→4*) TS for 1,5 H-shift

1	1.026606	-1.567300	-0.087713
6	-0.225020	-1.673214	-0.475297
1	-0.187140	-1.839712	-1.554017
6	-0.710441	-0.312442	-0.029021
1	-0.639594	-2.513575	0.082898
6	0.238652	0.803377	-0.568725
8	-0.658170	-0.233894	1.406657
6	-2.164041	-0.042886	-0.427712
1	-2.295905	-0.137469	-1.509304
1	-2.436952	0.973145	-0.130831
1	-2.826178	-0.752021	0.074961
8	-0.026062	2.013804	0.107795
1	0.038047	0.991275	-1.630030
6	1.732878	0.336185	-0.427031
8	1.888064	-0.828810	0.362049
1	2.278445	1.142014	0.076686
1	2.174302	0.189138	-1.424324
1	0.248807	-0.504488	1.638596
1	-0.243257	1.744076	1.017794

A2(2→3,3→4*)

1	0.051550	1.932173	-1.134849
6	-0.069915	1.906864	-0.048509
1	0.909566	2.076592	0.413102
6	-0.703083	0.576818	0.391778
1	-0.727401	2.728117	0.248153
6	0.047535	-0.645018	-0.186693
8	-2.044788	0.502019	-0.099705
6	-0.815676	0.490359	1.914384
1	0.157871	0.599839	2.401849
1	-1.258319	-0.463523	2.215701
1	-1.468148	1.291641	2.271810
8	-0.069547	-0.577202	-1.600127
1	-0.460623	-1.546948	0.191409
6	1.544642	-0.762779	0.175211
8	2.166173	-1.726116	-0.576303
1	1.731418	-0.887768	1.254352
1	2.051311	0.179050	-0.125372
1	-1.972632	0.340000	-1.052553
1	0.549678	-1.236248	-1.951542

A2(2→3,3→4*) TS for scission

1	0.999088	-1.109959	1.791278
6	1.268992	-0.095198	1.486083
1	0.657942	0.602770	2.066782

6	1.063330	0.094667	-0.020723
1	2.320319	0.078801	1.729703
6	-0.334968	-0.283105	-0.470905
8	1.962589	-0.766787	-0.752072
6	1.411556	1.511898	-0.471632
1	0.797704	2.255389	0.044341
1	1.265789	1.619302	-1.550334
1	2.462737	1.713712	-0.250466
8	-0.747991	-1.494002	-0.023722
1	-0.578056	-0.045816	-1.509970
6	-1.956515	0.869308	0.245752
8	-2.883691	0.119023	-0.132176
1	-1.743863	1.821616	-0.274863
1	-1.572750	0.821381	1.282534
1	1.744777	-1.677530	-0.505161
1	-1.715313	-1.530959	-0.171545

A2(2→4*)

1	0.136212	2.189097	-1.600069
6	0.311192	2.139066	-0.521420
1	1.382122	2.252728	-0.331430
6	-0.194682	0.802703	0.029610
1	-0.224032	2.968010	-0.050476
6	0.660427	-0.349736	-0.590994
8	-1.546086	0.677725	-0.405559
6	-0.128599	0.785984	1.564865
1	0.874632	1.020702	1.934989
1	-0.435836	-0.188283	1.963212
1	-0.816470	1.541211	1.953741
8	1.882922	-0.567927	0.050868
1	0.906951	-0.115716	-1.631906
6	-0.196348	-1.721168	-0.716437
8	-0.839828	-1.946584	0.443267
1	0.552907	-2.486050	-0.976235
1	-0.878852	-1.524893	-1.560041
1	-1.891228	-0.127109	0.016999
1	1.705587	-0.776504	0.978875

A2(2→4*) H-atom transfer

1	-1.827607	-0.217791	-1.858223
6	-2.014008	-0.107996	-0.787095
1	-2.384917	0.901014	-0.589083
6	-0.716629	-0.360101	0.004105
1	-2.774521	-0.836191	-0.492444
6	0.333513	0.756868	-0.442647
8	-0.172373	-1.568629	-0.399441

6	-0.971075	-0.328294	1.520860
1	-1.381380	0.633582	1.849960
1	-0.058492	-0.538192	2.086156
1	-1.701193	-1.100863	1.776420
8	-0.040954	2.058449	-0.109541
1	0.392315	0.715670	-1.533637
6	1.736093	0.359919	0.140246
8	2.013762	-0.950815	-0.171337
1	1.731753	0.561864	1.227638
1	2.466007	1.030155	-0.337371
1	0.976864	-1.522229	-0.155184
1	-0.049677	2.138571	0.855504

A2(3→4*)

1	-1.420640	1.431775	-0.220339
6	-0.692808	1.430472	0.596858
1	0.132378	2.095272	0.329886
6	-0.176027	0.021220	0.881593
1	-1.188894	1.827703	1.486729
6	0.526282	-0.605075	-0.361726
8	-1.337737	-0.770408	1.183550
6	0.793567	0.021517	2.068294
1	1.693289	0.593515	1.831265
1	1.107812	-1.001521	2.312991
1	0.312629	0.452713	2.951128
1	0.823042	-1.626927	-0.083222
8	1.699254	0.092593	-0.726706
6	-0.418470	-0.683512	-1.585068
8	-0.438882	0.483409	-2.303756
1	-1.424208	-1.043910	-1.324707
1	0.011324	-1.422687	-2.295664
1	1.410703	0.740181	-1.392646
1	-1.033772	-1.598597	1.580161

A2(3→4*) TS for scission

1	-0.322163	-1.074912	1.550278
6	0.619218	-0.529382	1.469818
1	0.547252	0.376792	2.078503
6	0.927930	-0.177351	0.014355
1	1.430014	-1.145090	1.867049
6	-0.169683	0.652310	-0.655373
8	1.067939	-1.420907	-0.682505
6	2.242588	0.626997	-0.082045
1	2.149483	1.590539	0.426141
1	2.506356	0.824264	-1.128386
1	3.055975	0.056680	0.376803

1	-0.022718	0.829268	-1.724558
8	-0.659717	1.749694	-0.030086
6	-1.965535	-0.586302	-0.592536
8	-2.371739	-0.331354	0.556853
1	-1.440792	-1.527024	-0.827902
1	-2.362310	-0.034666	-1.467399
1	-1.190055	1.441937	0.730129
1	1.429989	-1.234884	-1.560070

A2(3→4*) TS for 1,5 H-shift

1	-0.927928	-0.916113	1.125167
6	0.360709	-0.760499	1.320361
1	0.393525	-0.080088	2.171190
6	0.839419	-0.172190	0.008336
1	0.760860	-1.751177	1.535458
6	-0.345127	0.609284	-0.656979
8	1.184115	-1.287346	-0.823621
6	2.052305	0.751895	0.204863
1	1.776122	1.627883	0.794641
1	2.418085	1.104151	-0.767976
1	2.863547	0.214132	0.702829
1	-0.034280	0.942036	-1.656822
8	-0.686584	1.762371	0.088705
6	-1.557116	-0.334105	-0.739384
8	-1.983010	-0.621997	0.574170
1	-1.308432	-1.238090	-1.309165
1	-2.384759	0.191414	-1.235602
1	-1.330261	1.452082	0.747843
1	1.556213	-0.936763	-1.644771

A2(2→3)

1	0.293453	1.909804	-1.156791
6	0.059987	1.810595	-0.093902
1	0.986904	1.901381	0.480142
6	-0.644048	0.475517	0.174708
1	-0.585799	2.645515	0.203335
6	0.109732	-0.722234	-0.463022
8	-1.900178	0.445197	-0.543931
6	-0.904847	0.257282	1.666522
1	0.028045	0.172116	2.230099
1	-1.481172	-0.659224	1.819413
1	-1.478682	1.096191	2.077864
8	0.117856	-0.601519	-1.876404
1	-0.417646	-1.637538	-0.149290
6	1.584381	-0.858660	-0.059638
8	1.833380	-1.147705	1.249326

1	2.181025	0.005034	-0.408541
1	2.003931	-1.708820	-0.640747
1	-2.389088	1.250023	-0.327953
1	-0.780659	-0.317265	-2.107464

A2(3→2)

1	0.236595	1.808403	-1.329192
6	0.028446	1.801906	-0.256430
1	0.967862	1.947356	0.283721
6	-0.643766	0.489630	0.148505
1	-0.635993	2.638015	-0.024507
6	0.113632	-0.754663	-0.398542
8	-1.921075	0.501558	-0.538387
6	-0.866628	0.406672	1.658312
1	0.082561	0.370199	2.198994
1	-1.421669	-0.502074	1.922011
1	-1.439125	1.273380	2.001823
8	0.058953	-0.770181	-1.813948
1	-0.379301	-1.649326	0.024568
6	1.604457	-0.837031	-0.037918
8	1.896338	-1.003255	1.283388
1	2.175078	-0.002466	-0.485811
1	2.016110	-1.734857	-0.549304
1	-2.470568	-0.191213	-0.143984
1	-0.822128	-0.421472	-2.030312

A3(3→4,4→2*)

1	0.875525	1.979380	-1.229503
6	0.743380	2.065844	-0.151281
1	1.728133	2.108946	0.324982
6	-0.088199	0.881103	0.377133
1	0.214356	2.997767	0.070801
6	0.759414	-0.516881	-0.000470
8	-1.253977	0.726533	-0.271556
6	-0.248658	0.930307	1.911418
1	0.718868	0.900846	2.423021
1	-0.871208	0.109993	2.275620
1	-0.744062	1.867447	2.182820
1	1.611595	-0.481100	0.687823
8	1.241691	-0.488023	-1.296992
6	-0.125392	-1.752499	0.200562
8	-1.055391	-1.841176	-0.866296
1	-0.615745	-1.747044	1.180599
1	0.507482	-2.644200	0.138663
1	-1.645144	-1.070190	-0.756645

1	0.518348	-0.847766	-1.843603

A3(3→4,4→2*) TS for scission

1	1.493068	1.897348	0.675505
6	1.993825	1.037976	0.228371
1	2.369631	1.308860	-0.762923
6	1.073807	-0.188042	0.207104
1	2.858350	0.783702	0.854819
6	-0.557188	0.471913	-0.814540
8	0.497837	-0.504027	1.303762
6	1.558869	-1.316709	-0.708504
1	1.876572	-0.953054	-1.690204
1	0.797153	-2.088567	-0.832357
1	2.424621	-1.787261	-0.227913
1	-0.134599	0.585255	-1.813664
8	-0.896186	1.659341	-0.264404
6	-1.621423	-0.594611	-0.596027
8	-2.085733	-0.517652	0.738438
1	-1.260809	-1.594630	-0.862891
1	-2.479953	-0.368637	-1.244254
1	-1.304418	-0.770093	1.277220
1	-1.454296	1.422620	0.505863

A3(4→3,3→2*)

1	0.896454	2.109187	-1.143950
6	0.566004	2.197158	-0.109245
1	1.436851	2.251020	0.550391
6	-0.265085	0.930954	0.297545
1	-0.038034	3.097625	0.016456
6	0.534869	-0.342346	-0.124656
8	-1.393767	1.017611	-0.484392
6	-0.605331	0.987012	1.795624
1	0.296095	0.866940	2.405628
1	-1.313190	0.199128	2.064358
1	-1.064331	1.949329	2.036805
1	1.559120	-0.295286	0.262332
8	0.638093	-0.378077	-1.544634
6	-0.123269	-1.649087	0.343727
8	0.552395	-2.757784	-0.208173
1	-1.188686	-1.626398	0.047935
1	-0.080259	-1.751710	1.432347
1	0.713786	-2.516082	-1.134273
1	-0.234698	-0.079905	-1.858415

A3(4→3,3→2*) TS for scission

1	-1.697845	-1.862319	-0.522909

6	-2.056454	-0.845838	-0.689290
1	-2.013081	-0.610451	-1.756409
6	-1.261842	0.153130	0.163285
1	-3.104891	-0.792821	-0.372715
6	0.604501	-0.335345	-0.463360
8	-1.055363	-0.131169	1.387398
6	-1.456384	1.617481	-0.227520
1	-1.197265	1.810775	-1.273159
1	-0.876403	2.270236	0.427446
1	-2.516077	1.872543	-0.100192
1	0.561530	-0.380432	-1.553101
8	0.755495	-1.584544	0.073270
6	1.529113	0.716544	0.112493
8	2.870685	0.392030	-0.232053
1	1.376477	0.776005	1.199265
1	1.328332	1.697635	-0.322242
1	3.029390	-0.506650	0.091269
1	0.389685	-1.520893	0.980178

A3(3→2*)

1	1.021036	1.946803	-1.417298
6	0.633791	2.079324	-0.407510
1	1.465660	2.155394	0.298815
6	-0.222712	0.829234	-0.002480
1	0.028178	2.985923	-0.351526
6	0.604505	-0.456603	-0.359396
8	-1.315743	0.897910	-0.833766
6	-0.644503	0.948918	1.472256
1	0.203224	0.768086	2.140133
1	-1.441637	0.235254	1.703984
1	-1.042360	1.947983	1.669234
1	1.609018	-0.374672	0.071885
8	0.744722	-0.515393	-1.767186
6	-0.014331	-1.775850	0.145733
8	0.220167	-2.034444	1.523841
1	0.476752	-2.579308	-0.409681
1	-1.086061	-1.806673	-0.106731
1	-0.444495	-1.566807	2.041625
1	-0.122990	-0.246708	-2.115170

A3(4→2*)

1	0.403713	1.846507	-1.135724
6	0.378920	1.829969	-0.043687
1	1.402908	1.810152	0.338341
6	-0.422205	0.619823	0.469921
1	-0.104471	2.752204	0.292995

6	0.418283	-0.766465	0.160529
8	-1.588552	0.432344	-0.185458
6	-0.632983	0.678939	1.997766
1	0.319249	0.779358	2.528625
1	-1.157740	-0.214876	2.348031
1	-1.247388	1.549186	2.245018
1	-0.202080	-1.572074	0.570584
8	1.679839	-0.700569	0.767187
6	0.603214	-0.992162	-1.343141
8	-0.625958	-1.193799	-1.995981
1	1.191529	-1.908061	-1.464147
1	1.191267	-0.168024	-1.773746
1	-1.191751	-0.429195	-1.775310
1	1.600750	-0.969603	1.691011

A3(3→4)

1	0.385562	2.041715	-1.072498
6	0.219455	1.979442	0.006674
1	1.189914	1.923648	0.504538
6	-0.629780	0.741049	0.358959
1	-0.302479	2.887328	0.318581
6	0.104143	-0.602871	0.103006
8	-1.832663	0.753081	-0.308083
6	-1.036329	0.798870	1.867415
1	-0.120653	0.713580	2.457015
1	-1.701908	-0.031660	2.113220
1	-1.540360	1.742250	2.084635
1	-0.565761	-1.406559	0.449581
8	1.318270	-0.609506	0.838784
6	0.389098	-0.859344	-1.374196
8	1.092087	-2.104831	-1.418468
1	1.008177	-0.050980	-1.786614
1	-0.555879	-0.903406	-1.932245
1	1.479087	-2.208219	-2.295998
1	1.823224	-1.360531	0.490778

A3(4→3)

1	0.183647	2.024285	-1.196725
6	0.171244	1.987930	-0.104401
1	1.203891	1.966366	0.253237
6	-0.604537	0.751770	0.385916
1	-0.314505	2.899340	0.254758
6	0.130784	-0.600287	0.089943
8	-1.871143	0.682674	-0.140703
6	-0.840624	0.847195	1.926007
1	0.135358	0.900410	2.417942

1	-1.394396	-0.022562	2.287825
1	-1.404048	1.751563	2.163876
1	-0.486024	-1.405310	0.510986
8	1.447549	-0.626599	0.649281
6	0.303847	-0.879016	-1.401522
8	0.897504	-2.147130	-1.609555
1	0.901923	-0.078048	-1.862008
1	-0.679471	-0.890731	-1.881073
1	1.709371	-2.138687	-1.081851
1	1.388695	-0.923738	1.565190