
Electronic Supplementary Information for PCCP Article

**Multi-Structural Variational Transition State Theory: Kinetics of the
1,5-Hydrogen Shift Isomerization of 1-Butoxyl Radical Including All
Structures and Torsional Anharmonicity**

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Contents:

The coordinates (in Å) of ten structures (five pairs of mirror images) of 1-butoxyl radical (for each pair of mirror images, the coordinates are given for only one structure)

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The coordinates (in Å) of 37 structures (18 pairs of mirror images and one symmetric structure with a mirror plane) of 4-hydroxy-1-butyl radical (for each pair of mirror images, the coordinates are given for only one structure)

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The coordinates (in Å) of two structures (one pair of mirror images) of transition state (the coordinates are given for only one of them)

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Modified MM3 parameters

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Reactant 1-butoxyl

G^-T^+, G^+T^-

6	2.3394451	-0.1203832	-0.1368344
6	0.9040921	-0.3505202	0.3392877
6	-0.0610547	0.7108703	-0.1924915
6	-1.5070423	0.4181467	0.2061123
8	-2.0015519	-0.7664739	-0.2622879
1	3.0225062	-0.8837811	0.2538429
1	2.3940359	-0.1489204	-1.2331781
1	-2.2041788	1.2352433	-0.0683283
1	0.5497952	-1.3390666	0.0149102
1	0.8696395	-0.3508896	1.4399928
1	0.2222087	1.7069463	0.1810809
1	-0.0017253	0.7524483	-1.2905132
1	-1.6014634	0.3497541	1.3152697
1	2.7089553	0.8613751	0.1887811

G^-G^-, G^+G^+

6	1.7404362	-0.6685296	0.312009
6	1.0462182	0.3671245	-0.5780695
6	-0.1445816	1.0419947	0.1114208
6	-1.241452	0.0449727	0.5027511
8	-1.6594955	-0.7692683	-0.5090715
1	2.6524023	-1.0509943	-0.1609728
1	2.0218694	-0.2310526	1.2804797
1	-2.1027983	0.53249	0.9981529
1	1.7665676	1.1403331	-0.87746
1	0.694956	-0.1152575	-1.4999585
1	0.1870738	1.5659224	1.0212474
1	-0.5844543	1.7995445	-0.5519579
1	-0.8532916	-0.668888	1.2682772
1	1.0899143	-1.5313249	0.5060957

g^-G^+, g^+G^-

6	1.4981316	-0.8933601	-0.0330126
6	1.2158516	0.5930669	0.1967239
6	-0.1456602	1.033094	-0.3550793
6	-1.3000794	0.262879	0.2987236
8	-1.4452194	-1.0215547	-0.1449583
1	2.494355	-1.1691746	0.3332847
1	0.7642432	-1.5259388	0.4862493

	1	-2.2669026	0.739024	0.0123033
	1	1.2550846	0.8166555	1.2741156
	1	2.0034236	1.1983043	-0.2736395
	1	-0.2923673	2.1082878	-0.180617
	1	-0.1924281	0.8597004	-1.4399082
	1	-1.2552186	0.3132794	1.4044919
	1	1.4421034	-1.1417796	-1.1007477
T^-T^-, T^+T^+				
	6	2.4535568	-0.2580903	8.506E-05
	6	1.1405008	0.527397	0.0097852
	6	-0.0833545	-0.3914535	-0.0089486
	6	-1.389751	0.4001461	-0.015711
	8	-2.5349255	-0.340937	0.0084141
	1	3.3244157	0.4077015	0.0142906
	1	2.518146	-0.9185283	0.8747209
	1	-1.4332955	1.1177946	-0.862168
	1	1.0991704	1.1722839	0.9012608
	1	1.1044906	1.2016488	-0.8597757
	1	-0.0552975	-1.036727	-0.8992242
	1	-0.0755959	-1.0561517	0.8668609
	1	-1.4516686	1.0587594	0.8823939
	1	2.5233256	-0.8872816	-0.8969357
T^-G^-, T^+G^+				
	6	1.9422887	-0.7059156	-0.1602153
	6	1.2837411	0.6109808	0.2639472
	6	-0.1460471	0.761148	-0.2683969
	6	-1.0796763	-0.3252278	0.2753066
	8	-2.377313	-0.2192707	-0.1288103
	1	2.9936906	-0.7440761	0.147856
	1	1.4406862	-1.5741063	0.2877099
	1	-1.0047506	-0.4192235	1.3780631
	1	1.2738163	0.683672	1.3623501
	1	1.8872705	1.4554868	-0.0944288
	1	-0.5569087	1.7384614	0.0185766
	1	-0.154296	0.7164463	-1.3668541
	1	-0.768715	-1.3235993	-0.1147616
	1	1.9058722	-0.8248084	-1.2518786

Product, 4-hydroxy-1-butyl

$G^-G^+G^-T^+, G^+G^-G^+T^-$

6	1.5743682	0.8890043	-0.0808677
6	1.2505703	-0.5312019	0.2442920
6	-0.0697392	-1.0270477	-0.3707773
6	-1.3000065	-0.3610278	0.2458099
8	-1.4103786	1.0122085	-0.0803498
1	1.3771106	1.2748937	-1.0806183
1	2.1874596	1.4939457	0.5828464
1	2.0698116	-1.1814719	-0.1183010
1	1.2240505	-0.6745345	1.3359433
1	-0.1502874	-2.1138110	-0.2265740
1	-0.0703136	-0.8386331	-1.4548708
1	-1.2837650	-0.5003856	1.3417901
1	-2.2138786	-0.8357989	-0.1317469
1	-0.5883159	1.4597659	0.1635876

$G^-G^+G^+T^-, G^+G^-G^-T^+$

6	-1.7118306	-0.6944432	0.4200424
6	-1.1364193	0.2629270	-0.5687288
6	0.0381796	1.0784105	-0.0061098
6	1.1481140	0.1807464	0.5449020
8	1.6016767	-0.7620431	-0.4125800
1	-1.6723828	-0.4774893	1.4866938
1	-2.3230085	-1.5352576	0.1014915
1	-0.8101453	-0.2739981	-1.4734658
1	-1.9185014	0.9609355	-0.9212622
1	-0.3171576	1.7344739	0.8032626
1	0.4485425	1.7213985	-0.7959897
1	0.7989407	-0.3366272	1.4538351
1	2.0208045	0.7831284	0.8236410
1	0.9312318	-1.4460632	-0.5182008

$T^+G^-G^-T^+, T^-G^+G^+T^-$

6	1.8729536	-0.6285899	0.3886089
6	1.1178558	0.1555600	-0.6305459
6	0.0007240	1.0071588	-0.0093510
6	-1.0897918	0.1427380	0.6090459
8	-1.6847207	-0.6129079	-0.4373369
1	2.0007016	-0.2406890	1.3989037
1	2.4099185	-1.5359547	0.1255740
1	1.8063206	0.8210898	-1.1841308
1	0.6794629	-0.5164769	-1.3820687

	1	-0.4540699	1.6519097	-0.7735478
	1	0.4196659	1.6616627	0.7697908
	1	-1.8417016	0.7756168	1.1066518
	1	-0.6447079	-0.5268689	1.3648437
	1	-2.3082765	-1.2482247	-0.073869
$G^-G^-G^-T^+, G^+G^+G^+T^-$				
	6	1.9098916	-0.5934789	0.3589169
	6	1.1074298	0.1656630	-0.6429109
	6	-0.0119450	0.9901648	0.009655
	6	-1.0834318	0.0975980	0.6343839
	8	-1.7199717	-0.7270379	-0.3299889
	1	2.0493956	-0.2001460	1.3652837
	1	2.4538605	-1.4940077	0.088005
	1	1.7625736	0.8429728	-1.2218618
	1	0.6653549	-0.5258399	-1.3753537
	1	-0.4811289	1.6516697	-0.7355139
	1	0.4114249	1.6414137	0.7900108
	1	-1.8244206	0.7047049	1.1784398
	1	-0.6208019	-0.5902059	1.3548187
	1	-2.1881546	-0.173941	-0.9641938
$T^+G^-T^+T^+, T^-G^+T^-T^-$				
	6	2.4133305	-0.152537	-0.148887
	6	1.0144198	-0.3490129	0.3246179
	6	0.059174	0.7421719	-0.1737990
	6	-1.3766897	0.4976529	0.2661230
	8	-1.8077306	-0.7265969	-0.3125019
	1	2.6148275	0.4045139	-1.0619238
	1	3.2485793	-0.6519079	0.3349799
	1	0.6225689	-1.3260487	-0.0121020
	1	0.9867118	-0.3872519	1.4265487
	1	0.088071	0.7809208	-1.2728867
	1	0.3855869	1.7246237	0.1963350
	1	-2.0203086	1.3294087	-0.061533
	1	-1.4236697	0.4419909	1.3674277
	1	-2.7019275	-0.9331268	-0.0251610
$T^+G^-T^-T^-, T^-G^+T^+T^+$				
	6	2.4199035	-0.155063	-0.1278720
	6	1.0077528	-0.3696489	0.2959709
	6	0.0623330	0.7276599	-0.2058180
	6	-1.3706257	0.5104949	0.2568170
	8	-1.8218066	-0.7225319	-0.2867389

	1	2.7635974	0.8285388	-0.4426919
	1	3.1565764	-0.9510708	-0.0578960
	1	0.6422509	-1.3472317	-0.0524700
	1	0.9413138	-0.4127299	1.4015807
	1	0.0800430	0.7559299	-1.3047387
	1	0.4069899	1.7092987	0.1522190
	1	-2.0092396	1.3413307	-0.0827070
	1	-1.4040277	0.4811659	1.3597367
	1	-2.7192344	-0.9056408	0.0062910
$G^-G^-T^+T^-, G^+G^+T^-T^+$				
	6	2.4132432	-0.1607127	-0.1539729
	6	1.0156563	-0.3391968	0.3305380
	6	0.0524646	0.7213467	-0.2141287
	6	-1.3814225	0.5028231	0.2617517
	8	-1.9009065	-0.7521216	-0.1512522
	1	2.7507954	0.8004252	-0.5373840
	1	3.1506769	-0.9523417	-0.0503783
	1	0.6390178	-1.3401893	0.0697704
	1	0.9847723	-0.3026723	1.4374232
	1	0.0770341	0.7103422	-1.3162834
	1	0.3857507	1.7236357	0.0957716
	1	-2.0309107	1.3243791	-0.0801568
	1	-1.4148446	0.4904945	1.3593684
	1	-1.9346897	-0.7826623	-1.1132420
$G^-G^-T^+T^+, G^+G^+T^-T^-$				
	6	2.4070430	-0.1583771	-0.1682679
	6	1.0209457	-0.3184778	0.3538370
	6	0.0497421	0.7350852	-0.1906441
	6	-1.3863139	0.4925693	0.2673930
	8	-1.8866542	-0.7626003	-0.1678762
	1	2.5915132	0.3740731	-1.0994075
	1	3.2503062	-0.6482228	0.3113057
	1	0.6216107	-1.3187285	0.1034998
	1	1.0212461	-0.2791157	1.4559886
	1	0.0840250	0.7302125	-1.2932874
	1	0.3668035	1.7393988	0.1269727
	1	-2.0420191	1.3110509	-0.0699366
	1	-1.4310535	0.4651589	1.3642705
	1	-1.9176989	-0.7778226	-1.1303040
$T^+T^-G^+T^-, T^-T^+G^-T^+$				
	6	2.0303206	-0.7460089	-0.1788470

	6	1.4170457	0.5506749	0.2311070
	6	-0.0219080	0.7139819	-0.2770099
	6	-0.9531718	-0.3175509	0.3424029
	8	-2.2554255	-0.1089370	-0.1806870
	1	1.7242297	-1.2264568	-1.1072568
	1	2.8750774	-1.1702578	0.3572029
	1	1.4394847	0.6499829	1.3285537
	1	2.0244216	1.3930747	-0.1489070
	1	-0.0486220	0.6006189	-1.3707287
	1	-0.4028969	1.7175507	-0.0463480
	1	-0.9475418	-0.2052350	1.4406867
	1	-0.5904979	-1.3327557	0.1084350
	1	-2.8639764	-0.7616088	0.1779390
$G^-T^-G^+T^+, G^+T^+G^-T^-$				
	6	2.0424116	-0.7248039	-0.1634950
	6	1.4082837	0.5706809	0.2169640
	6	-0.0327180	0.6953469	-0.2979339
	6	-0.9518428	-0.3369779	0.3505349
	8	-2.2763695	-0.2830079	-0.1494740
	1	1.7262187	-1.2460908	-1.0659148
	1	2.9040964	-1.1135748	0.3722599
	1	1.4242197	0.6928329	1.3124267
	1	2.0036466	1.4147747	-0.1779100
	1	-0.0553880	0.5545709	-1.3886187
	1	-0.4182299	1.7061157	-0.093262
	1	-0.9381338	-0.210762	1.4474797
	1	-0.5858719	-1.3497297	0.138067
	1	-2.6464105	0.5904509	0.014836
$G^-T^-G^-T^+, G^+T^+G^+T^-$				
	6	-2.0308456	-0.7435779	-0.1658640
	6	-1.4145787	0.5632419	0.2052510
	6	0.0303250	0.7019819	-0.2959259
	6	0.9580248	-0.3031039	0.3823039
	8	2.3039215	-0.1810030	-0.0443370
	1	-1.7344607	-1.2475088	-1.0849828
	1	-2.8656454	-1.1584118	0.3923159
	1	-2.0154856	1.3957537	-0.2056810
	1	-1.4412577	0.6981839	1.2984617
	1	0.4099919	1.7158287	-0.1126070
	1	0.0522240	0.5394319	-1.3865967
	1	0.5824619	-1.3283577	0.2232510

	1	0.9660788	-0.1263760	1.4661927
	1	2.3571615	-0.3517649	-0.9902468
$G^-G^+T^+T^-$, $G^+G^-T^-T^+$				
	6	-2.4200662	-0.1225920	-0.1357803
	6	-1.0103920	-0.3710362	0.2794766
	6	-0.0529870	0.7443053	-0.1590448
	6	1.3870487	0.4917007	0.2812563
	8	1.9476133	-0.6656041	-0.3181593
	1	-2.6366778	0.5060334	-0.9970481
	1	-3.2485005	-0.6423299	0.3378597
	1	-0.9533014	-0.4999594	1.3736442
	1	-0.6639138	-1.3315497	-0.1521887
	1	-0.3927671	1.7016900	0.2628899
	1	-0.0795222	0.8408098	-1.2543466
	1	1.4366989	0.4201852	1.3817110
	1	2.0283123	1.3272790	-0.0226131
	1	1.5071447	-1.4515922	0.0199184
$G^-G^+T^+T^+$, $G^+G^-T^-T^-$				
	6	-2.4252617	-0.1281368	-0.1127409
	6	-1.0037769	-0.3840376	0.2553738
	6	-0.0549822	0.7296018	-0.2051146
	6	1.3811886	0.5091282	0.2635962
	8	1.9589806	-0.6673118	-0.2796809
	1	-2.7683402	0.8832955	-0.3204113
	1	-3.1641792	-0.9248074	-0.1000261
	1	-0.9080290	-0.4980807	1.3544396
	1	-0.6842551	-1.3500665	-0.1706965
	1	-0.4116500	1.6940148	0.1879942
	1	-0.0700572	0.7971067	-1.3020278
	1	1.4158324	0.4827708	1.3667641
	1	2.0199519	1.3367948	-0.0659165
	1	1.5158747	-1.4418678	0.0806404
$G^-T^-T^+T^+$, $G^+T^+T^-T^-$				
	6	-2.5445485	-0.3196539	0.0045660
	6	-1.2949827	0.4927979	0.0081850
	6	-0.023893	-0.3642899	0.0026010
	6	1.2402768	0.4893149	-0.0185470
	8	2.4255835	-0.2851209	-0.0688330
	1	-2.5362595	-1.3442937	-0.3613919
	1	-3.5027283	0.1192890	0.2693939
	1	-1.2727127	1.1622178	-0.8741078

	1	-1.2854587	1.1682688	0.8796058
	1	-0.0212300	-1.0274858	-0.8745028
	1	-0.0160110	-1.0114128	0.8944378
	1	1.2506878	1.1672688	0.8525678
	1	1.2519977	1.1179968	-0.9186158
	1	2.4659255	-0.8599048	0.7024479
$T^+T^+T^+, T^+T^+T^+$				
	6	-2.5484315	-0.3089199	-0.0065780
	6	-1.2948047	0.4972679	0.0105480
	6	-0.030623	-0.3672039	-0.0226700
	6	1.2351518	0.4741199	0.0179980
	8	2.3510885	-0.4010089	-0.0134550
	1	-2.5236025	-1.3778737	0.1936790
	1	-3.5172593	0.1613250	-0.1527520
	1	-1.2868797	1.2008988	-0.8398978
	1	-1.2688237	1.1398378	0.9120558
	1	-0.019059	-0.9841038	-0.9320678
	1	-0.024952	-1.0571698	0.8333298
	1	1.2435137	1.0872858	0.9355968
	1	1.2516897	1.1616478	-0.8450928
	1	3.1689044	0.1046490	0.0069980
$G^+T^+T^+, G^+T^+T^+$				
	6	2.5446115	-0.3195029	-0.014007
	6	1.2949427	0.4913689	0.035116
	6	0.0241230	-0.3603859	-0.053139
	6	-1.2401117	0.4892139	0.031035
	8	-2.4261545	-0.2756749	-0.092680
	1	2.5149515	-1.3961107	0.1395250
	1	3.5159093	0.1516410	-0.1389270
	1	1.2641827	1.0878338	0.9675468
	1	1.2952327	1.2369778	-0.7783858
	1	0.0242430	-1.0980988	0.7663288
	1	0.0134170	-0.9272878	-0.9945818
	1	-1.2603607	1.2127548	-0.7944728
	1	-1.2418367	1.0675858	0.9713588
	1	-2.4578885	-0.9340658	0.6090209
$G^-G^-g^+G^+, G^+G^+g^-G^-$				
	6	1.6571147	0.7890988	0.1394611
	6	1.1672050	-0.5201227	-0.3846088
	6	-0.0897244	-1.0327199	0.3550327
	6	-1.3647721	-0.3309437	-0.1082431

	8	-1.2632603	1.0823625	-0.0794433
	1	1.6968693	1.6797040	-0.4804206
	1	2.0129239	0.8627495	1.1665560
	1	0.9437802	-0.4416563	-1.4577118
	1	1.9604631	-1.2794013	-0.2792594
	1	0.0429003	-0.8866902	1.4397203
	1	-0.2132677	-2.1134113	0.1954276
	1	-2.2217484	-0.6698747	0.4969153
	1	-1.5729247	-0.5964967	-1.1539533
	1	-0.7618532	1.3543015	0.6984208
TTTg ⁺ , TTTg ⁻				
	6	-2.5257097	0.4954342	0.0000000
	6	-1.3341928	-0.4016744	0.0000000
	6	0.0000000	0.3758247	0.0000000
	6	1.1926065	-0.5687412	0.0000000
	8	2.3770814	0.2116847	0.0000000
	1	-2.9347474	0.8811532	0.9304928
	1	-2.9347474	0.8811532	-0.9304928
	1	-1.3555512	-1.0583938	0.8835778
	1	-1.3555512	-1.0583938	-0.8835778
	1	0.0581453	1.0263711	0.8833178
	1	0.0581453	1.0263711	-0.8833178
	1	1.1505412	-1.2182475	-0.8911788
	1	1.1505412	-1.2182475	0.8911788
	1	3.1503493	-0.3603036	0.0000000
T ⁺ G ⁻ g ⁺ T ⁺ , T ⁻ G ⁺ g ⁻ T ⁻				
	6	-1.6559947	0.9175108	-0.0948480
	6	-1.2785607	-0.4795789	0.2707109
	6	0.0124520	-0.9898938	-0.3907409
	6	1.2908737	-0.4223799	0.2126840
	8	1.3718047	0.9650948	-0.0843430
	1	-0.9130068	1.6118157	-0.4749309
	1	-2.6599595	1.2821627	0.1093310
	1	-1.1657668	-0.5730599	1.3697077
	1	-2.1064926	-1.1597288	0.0138320
	1	-0.0023820	-0.7608088	-1.4662677
	1	0.0608580	-2.0837596	-0.2924459
	1	2.1626556	-0.9534398	-0.2027230
	1	1.2830447	-0.5830719	1.3047697
	1	2.1539956	1.3451827	0.3266409

Transition state

6	-1.3275053	-0.8738416	-0.0743752
6	-1.1711613	0.5960474	0.2475787
6	0.1525317	1.1110034	-0.338196
6	1.2934735	0.2563054	0.2333634
8	1.1268395	-1.095217	-0.0850784
1	-1.8813973	-1.4834381	0.6434766
1	-1.5964738	-1.0938153	-1.1119026
1	1.3575255	0.407394	1.3264813
1	-2.014798	1.175701	-0.1587559
1	-1.1682537	0.7493791	1.336008
1	0.1442554	1.0072343	-1.4329437
1	0.3139934	2.1693606	-0.095922
1	2.2518281	0.5720175	-0.2119585
1	-0.1054272	-1.2791848	-0.0240825

Modified MM3 parameters

Atom Type Definitions

atom	1	C	"CSP3 ALKANE"	6	12.000	4
atom	5	H	"EXCEPT ON N,O,S"	1	1.008	1
atom	6	O	"C-O-H, C-O-C, O-O"	8	15.995	2
atom	21	H	"-OH ALCOHOL"	1	1.008	1
atom	29	C*	"RADICAL"	6	12.000	3
atom	182	O*	"-C-O* radical"	8	15.995	1

#new van der Waals Parameters

vdw	1	1.640	0.027	
vdw	5	1.20	0.020	0.923
vdw	6	1.820	0.059	
vdw	21	1.100	0.016	0.923
vdw	29	1.5940	0.030	
vdw	182	1.500	0.059	

#new parameters for O* (-C-O* radical)

bond	1	182	5.7000	1.4130		
angle	1	1	182	0.830	107.500	107.000 107.900
angle	5	1	182	0.820	110.000	108.900 108.700
strbnd	182	0.100	0.090	0.000		
torsion	1	1	1	182	0.200 0.0 1	0.000 180.0 2 0.300 0.0 3
torsion	5	1	1	182	0.000 0.0 1	0.000 180.0 2 0.300 0.0 3
strtors	1	182	0.000	0.000	0.100	
dipole	1	182	1.1700	0.500		

#new parameters for H 21

bond	21	182	4.71	0.9707		
bond	21	1	4.7400	1.1120		
angle	21	1	5	0.550	107.600	107.800 109.470
angle	21	1	1	0.590	109.800	109.310 110.700
angle	21	182	1	0.750	106.800	0.000 0.000
torsion	1	1	1	21	0.200 0.0 1	0.000 180.0 2 0.300 0.0 3
torsion	5	1	1	21	0.000 0.0 1	0.000 180.0 2 0.300 0.0 3

#new parameters for C-H

bond	1	5	4.74	1.112 98
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