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

Supplementary Information for publication:

Radicals from tributyl phosphate decomposition: a combined electron paramagnetic resonance spectroscopy and computation chemistry

Ilya S. Sosulin, Delaney H. Ryan, Aliaksandra Lisouskaya*

Notre Dame Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556, USA

*Corresponding Author: alisousk@nd.edu; phone (574) 631-5457

Contents:

Table S1. Calculated molecular geometries and energies for conformers of TBP R1-R4 radicals at the DFT(B3LYP)/L1a_3 level of theory

Abbreviations:

E –energy,a.u.

R1-A

$molecule

mult=2

cartesian

set=L1a_3

15	0.86899558	-0.66531332	0.93664395
8	1.73501019	-1.27760156	1.96894918
8	1.60785700	-0.26651057	-0.44737281
8	-0.34474973	-1.54654047	0.39838662
8	0.16344654	0.71256964	1.32513710
6	2.53875022	-1.12753501	-1.01488788
6	3.05698984	-0.69271640	-2.33471205
6	1.99797216	-0.61326853	-3.45265693
6	1.40795361	-1.97076782	-3.83452248
6	-1.02964919	-2.49097589	1.26836297
6	-2.27833678	-1.88676504	1.88852374
6	-3.33459541	-1.44506562	0.87356547
6	-4.58555650	-0.86450503	1.53383616
6	0.83090972	1.67699489	2.18872360

6	1.46181979	2.82573429	1.41581443
6	0.49034625	3.82317046	0.76940925
6	-0.26794950	3.30719026	-0.45647575
1	3.09724323	-1.73933858	-0.31617107
1	3.85168661	-1.38836754	-2.62508581
1	3.53115963	0.29850065	-2.23529891
1	2.46208377	-0.15207904	-4.33126501
1	1.19703126	0.06256568	-3.13722018
1	0.91717273	-2.44438147	-2.98000836
1	2.18569588	-2.65411308	-4.19066340
1	0.66661673	-1.86699810	-4.63159468
1	-0.33002679	-2.83625707	2.03230479
1	-1.28130352	-3.33085693	0.61708706
1	-1.99383453	-1.04143352	2.52516844
1	-2.70230299	-2.64707661	2.55782404
1	-3.61373451	-2.30315140	0.24961049
1	-2.89909113	-0.70352839	0.19730912
1	-4.34099416	0.01516805	2.13721546
1	-5.06398732	-1.59469483	2.19422257
1	-5.32307121	-0.55900964	0.78687017
1	1.57811689	1.14853732	2.78459131
1	0.04801030	2.04117555	2.85821302
1	2.14643591	2.42104617	0.66232259

1 2.08675542 3.36522399 2.13894891

1 1.06452036 4.71042399 0.47990750

1 -0.22497878 4.16512524 1.52811180

1 -0.93043146 2.47698687 -0.20785927

1 0.42584539 2.95355635 -1.22492474

1 -0.87383150 4.10488207 -0.89634041

$end

Energy = -1115.5914199011

R1-B

$molecule

mult=2

cartesian

set=L1a_3

15 -0.49191168 -1.33461785 0.48407416

8 -0.94279054 -2.66427278 0.95139648

8 0.89371355 -1.31697150 -0.35288605

8 -1.46534311 -0.55996705 -0.51476718

8 -0.19686514 -0.24157577 1.60766164

6 1.20334582 -2.33895464 -1.23868843

6 2.27592766 -2.06452144 -2.22126735

6 1.82906702 -1.38971860 -3.54362391

6 1.27735316 0.02498076 -3.37221312

6 -2.90970518 -0.73058748 -0.43554803

6	-3.59876358	0.37860310	0.34537753
6	-3.62507828	1.76242417	-0.31875399
6	-2.29035593	2.51216264	-0.33516997
6	0.38995804	-0.62534325	2.88498153
6	1.88705816	-0.36221496	2.95296327
6	2.31525239	1.11100267	3.00821461
6	2.16030867	1.89338960	1.70130950
1	0.52297309	-3.17970104	-1.27215277
1	2.75292685	-3.01967388	-2.47094796
1	3.04272950	-1.44041564	-1.74568516
1	1.07873752	-2.02498071	-4.02728817
1	2.69495897	-1.36799004	-4.21614050
1	0.37926181	0.03480147	-2.75080101
1	1.01914109	0.46120216	-4.34157097
1	2.01408405	0.68098848	-2.89816114
1	-3.11686727	-1.70686440	0.00764054
1	-3.24415596	-0.74131865	-1.47560640
1	-3.15508493	0.44656965	1.34503614
1	-4.63270708	0.04133874	0.49272727
1	-4.36514148	2.37390260	0.20953521
1	-4.00152580	1.65737893	-1.34407659
1	-1.89402531	2.62549481	0.67820262
1	-2.41794291	3.51353096	-0.75683456

1 -1.53563733 1.99025058 -0.92490104

1 0.16905811 -1.67981496 3.06419207

1 -0.14516544 -0.02831606 3.62717623

1 2.38181897 -0.86968514 2.11775864

1 2.23663199 -0.86214704 3.86532359

1 3.36690012 1.14286870 3.31440578

1 1.75631580 1.61412075 3.80738314

1 1.11685477 1.97107090 1.39294410

1 2.70645384 1.40706421 0.88766315

1 2.55823598 2.90650703 1.81111711

$end

Energy = -1115.5870894833

R1-C

$molecule

mult=2

cartesian

set=L1a_3

15 0.37375806 -0.62722979 1.26849160

8 0.67939843 -1.00234500 2.66092134

8 1.34479775 -1.20788833 0.11166871

8 -1.04731981 -1.14939357 0.77084861

8 0.43166466 0.94259613 0.93665204

6 2.72547902 -1.19666116 0.26988153

6	3.47907957	-1.78876006	-0.86054494
6	3.35430265	-3.32567968	-0.98041597
6	4.14148398	-3.88541559	-2.16509238
6	-1.53996252	-0.90945483	-0.57275263
6	-2.99811629	-1.32507310	-0.63164742
6	-3.92946764	-0.48381423	0.24364090
6	-5.39221736	-0.91685993	0.13774079
6	-0.00904528	1.90398189	1.93472331
6	0.46773045	3.28336304	1.52140345
6	-0.12631221	3.79094764	0.20570435
6	0.34772154	5.19975222	-0.15339134
1	3.07544005	-1.23063244	1.29634782
1	4.53537550	-1.52340852	-0.73820274
1	3.14252737	-1.33134539	-1.79974423
1	2.29670756	-3.59030249	-1.07737441
1	3.70469633	-3.78489351	-0.04973225
1	3.78863600	-3.46204567	-3.11069623
1	4.04106491	-4.97228390	-2.22967208
1	5.20785544	-3.65470821	-2.07789132
1	-0.93564946	-1.49642407	-1.26835953
1	-1.42035286	0.15179409	-0.81046374
1	-3.07402298	-2.38180756	-0.35208369
1	-3.31191497	-1.25606913	-1.68096773

1 -3.83845161 0.57079395 -0.04473349

1 -3.60339776 -0.54962168 1.28587185

1 -5.51874428 -1.95752370 0.45115506

1 -5.75924543 -0.83431581 -0.89013269

1 -6.03538708 -0.30003891 0.77087073

1 0.40249450 1.61377435 2.90336511

1 -1.10221315 1.86662956 1.99122137

1 1.56178569 3.27316035 1.45957200

1 0.20706325 3.97198757 2.33511072

1 -1.22101708 3.78047733 0.27734379

1 0.13737993 3.09996652 -0.60065479

1 1.43592921 5.23394593 -0.26303376

1 0.07134797 5.92234051 0.62080810

1 -0.09088206 5.53848518 -1.09575581

$end

Energy = -1115.5947843785

R1-D

$molecule

mult=2

cartesian

set=L1a_3

15 -0.27226408 -0.76763957 1.31621787

8 -0.19149172 -1.46910684 2.61653410

8	1.13292719	-0.55101647	0.54331729
8	-1.13789369	-1.46919863	0.17473316
8	-0.85591832	0.71734796	1.34253256
6	2.12808209	-1.51856908	0.57930933
6	3.09442294	-1.47343271	-0.54135086
6	2.52818900	-1.94333978	-1.90190466
6	3.55971382	-1.85581247	-3.02660916
6	-2.34267526	-2.21779086	0.50480077
6	-3.61594683	-1.41200395	0.29304110
6	-3.99903862	-1.11872954	-1.16417039
6	-3.11745746	-0.09657080	-1.88679085
6	-0.57953532	1.60793410	2.46094958
6	0.63196854	2.48827622	2.20322485
6	0.49752062	3.40284537	0.98405051
6	1.72354856	4.29171710	0.77239201
1	1.93470438	-2.38761856	1.19568660
1	3.95422239	-2.09782488	-0.27340038
1	3.46992206	-0.44750194	-0.65452237
1	1.65334269	-1.33479386	-2.15035063
1	2.17239995	-2.97462149	-1.80216502
1	3.13862514	-2.19296904	-3.97773660
1	4.43554554	-2.47640879	-2.81243232
1	3.90911758	-0.82776646	-3.16365713

1 -2.26410358 -2.56151649 1.53849170

1 -2.31745116 -3.08951785 -0.15342038

1 -3.55015793 -0.47808147 0.86220215

1 -4.42172734 -1.99635478 0.75536676

1 -5.03413970 -0.75913515 -1.17223832

1 -4.00597627 -2.06126088 -1.72614012

1 -3.51255880 0.11196541 -2.88544714

1 -2.09037803 -0.44763939 -1.99580209

1 -3.08303208 0.84901109 -1.33743020

1 -0.45304658 1.00781353 3.36448139

1 -1.48617789 2.20842353 2.56216033

1 1.52327542 1.85940358 2.10361770

1 0.78204604 3.09438812 3.10654807

1 -0.39461796 4.03051419 1.10153680

1 0.32813196 2.79360201 0.09121587

1 2.62480486 3.69000147 0.62024310

1 1.90135849 4.93913063 1.63692127

1 1.60171940 4.93384742 -0.10400626

$end

Energy = -1115.5914871891

R2-A

$molecule

mult=2

cartesian

set=L1a_3

15	-0.00280956	-1.18757245	0.86683035
8	-0.23496170	-2.35938668	1.74552507
8	1.51767924	-0.92555106	0.43761234
8	-0.76280311	-1.20213053	-0.54118357
8	-0.43676920	0.23432730	1.46348147
6	2.40526133	-2.07671088	0.15012185
6	2.20633171	-2.62179096	-1.21236575
6	2.43714859	-1.81755505	-2.44771416
6	3.66875502	-0.90232790	-2.41752286
6	-2.10459640	-1.74756601	-0.65555305
6	-3.16273031	-0.65688957	-0.61897393
6	-3.05150291	0.36377113	-1.75334627
6	-4.14152244	1.43462690	-1.69743581
6	-0.20598396	0.54787753	2.86438050
6	1.00285314	1.44890145	3.07426501
6	0.85015101	2.90528401	2.61402174
6	0.81955444	3.11928103	1.09833212
1	2.23519884	-2.83392139	0.91616766
1	3.40025921	-1.64719805	0.28486406
1	1.69926091	-3.57638326	-1.30529287
1	1.54706528	-1.19447634	-2.63697275

1 2.50249886 -2.49704653 -3.30450987

1 3.58841355 -0.14396893 -1.63513199

1 3.77735579 -0.37971683 -3.37123009

1 4.58463795 -1.47412497 -2.24270752

1 -2.25800570 -2.48132426 0.13881218

1 -2.11405310 -2.26784400 -1.61644088

1 -3.12123639 -0.14591929 0.34909203

1 -4.13983080 -1.15602096 -0.66456365

1 -3.10242054 -0.16122307 -2.71543660

1 -2.06722097 0.83987452 -1.71567973

1 -4.09303041 1.99784049 -0.76040130

1 -5.14021631 0.99148084 -1.76443008

1 -4.03937347 2.14890343 -2.51886112

1 -0.09838820 -0.38733899 3.41868295

1 -1.12200809 1.04107637 3.19949300

1 1.87717337 0.99146371 2.59855971

1 1.20106500 1.44357969 4.15371689

1 1.68410268 3.47900255 3.03397659

1 -0.05815092 3.32669883 3.06324460

1 -0.04933643 2.64727676 0.63756292

1 1.71044674 2.69558296 0.62521042

1 0.79173825 4.18713848 0.86180040

$end

Energy = -1115.5875717222

R2-B

$molecule

mult=2

cartesian

set=L1a_3

15	0.72834859	-0.26729407	1.15743910
8	1.46040369	-0.81618537	2.32480305
8	1.63633352	0.30320703	-0.03212921
8	-0.24351254	-1.28546532	0.39560722
8	-0.24996536	0.96465070	1.45817326
6	2.90596782	-0.38077807	-0.37428310
6	2.70134985	-1.56203385	-1.24145655
6	2.22235595	-1.42633121	-2.64338121
6	2.39338623	-2.69448476	-3.48380777
6	-0.97028747	-2.30685041	1.13175151
6	-2.41786749	-1.92573501	1.40841179
6	-3.35587959	-1.89738176	0.19351012
6	-3.15261190	-0.72464505	-0.76942878
6	0.12668417	1.99083828	2.41666042
6	0.70161048	3.23858652	1.76114803
6	-0.28369657	4.09734762	0.95571122
6	-0.71815089	3.51403329	-0.39164313

1	3.40933925	-0.63839170	0.55819566
1	3.46717453	0.40405544	-0.88780384
1	2.74916829	-2.54888795	-0.79126960
1	2.73505941	-0.58082815	-3.12358977
1	1.15781696	-1.13918599	-2.63622075
1	3.44628322	-2.97934004	-3.56017902
1	2.00847009	-2.55088437	-4.49652011
1	1.85289654	-3.53436988	-3.03781229
1	-0.43585868	-2.51016688	2.06244888
1	-0.91830097	-3.19847666	0.50167046
1	-2.44401172	-0.96229478	1.92923823
1	-2.79311377	-2.67054397	2.12190888
1	-4.38655384	-1.87255859	0.56500960
1	-3.25829734	-2.84402727	-0.35299170
1	-3.90523855	-0.74432389	-1.56332841
1	-2.16668476	-0.74610671	-1.23545428
1	-3.24565463	0.23103854	-0.24522918
1	0.83706252	1.56027670	3.12626333
1	-0.79633791	2.22531182	2.95281893
1	1.55580833	2.95698365	1.13586907
1	1.10712050	3.84672718	2.57996961
1	0.18518120	5.07241779	0.78154231
1	-1.16853603	4.29763677	1.57319630

1 -1.26851051 2.57986335 -0.27296975

1 0.14954017 3.30359794 -1.02407220

1 -1.35829080 4.22099907 -0.92777635

$end

Energy = -1115.5862374967

R3-A

$molecule

mult=2

cartesian

set=L1a_3

15 -0.09899602 -0.73480125 1.29314756

8 -0.07004844 -1.49075512 2.56809062

8 1.31620965 -0.51960429 0.57556008

8 -0.97980343 -1.36743843 0.11732892

8 -0.66976014 0.75769424 1.37536827

6 2.32924030 -1.55876341 0.60690752

6 2.29005828 -2.42422985 -0.64493520

6 2.51891072 -1.68587965 -1.91826391

6 2.75831927 -2.42271039 -3.18822881

6 -2.26037346 -1.99328539 0.40644021

6 -3.44355747 -1.09248526 0.08206804

6 -3.71223729 -0.83703331 -1.40760564

6 -2.70650049 0.07677006 -2.11316580

6	-0.37096235	1.60558339	2.51764638
6	0.79770013	2.53748604	2.24143173
6	0.57192001	3.49914797	1.07303668
6	1.75560507	4.43893745	0.84122445
1	2.19515699	-2.15942437	1.50904655
1	3.27760760	-1.02248469	0.67573564
1	1.32484618	-2.95839516	-0.67528169
1	3.04853302	-3.21255146	-0.52343082
1	2.27355057	-0.63031139	-1.95666277
1	3.06682477	-1.75468806	-3.99578530
1	1.85195618	-2.94913542	-3.53281628
1	3.52897823	-3.19523528	-3.07063190
1	-2.27298853	-2.29372580	1.45672480
1	-2.27879370	-2.89620359	-0.20903317
1	-3.32802455	-0.14180886	0.61383908
1	-4.32393973	-1.58329783	0.51642313
1	-4.71145221	-0.39597908	-1.49711448
1	-3.76348756	-1.80075908	-1.93009181
1	-1.70661473	-0.35881556	-2.13803700
1	-2.62967493	1.04158038	-1.60288238
1	-3.01973921	0.26838956	-3.14379448
1	-0.18237083	0.97352313	3.38827905
1	-1.28901759	2.17191863	2.69111445

1 1.70098399 1.94303360 2.06664787

1 0.97592063 3.10872433 3.16224076

1 -0.33327259 4.08942316 1.26268337

1 0.37765887 2.92309683 0.16345749

1 2.66695284 3.87652431 0.61592051

1 1.95689455 5.05307705 1.72472625

1 1.56778740 5.11489185 0.00267203

$end

Energy = -1115.5894232857

R3-B

$molecule

mult=2

cartesian

set=L1a_3

15 -0.42847533 -1.32589893 0.61272474

8 -1.12094393 -2.40443859 1.35737988

8 1.13436182 -1.54526109 0.34374421

8 -0.97981722 -1.02342763 -0.85905013

8 -0.45300854 0.12239298 1.29204413

6 1.65145107 -2.85760071 0.00702983

6 1.89257089 -3.00285155 -1.50117779

6 2.89413462 -2.05220527 -2.06506258

6 2.50561689 -0.76685337 -2.70449663

6	-2.40551651	-1.06237340	-1.14015114
6	-3.02560684	0.32512487	-1.11471330
6	-2.44112615	1.29369555	-2.14484747
6	-3.10649549	2.66994312	-2.10925700
6	-0.36911516	0.26874829	2.73626942
6	1.06308457	0.47590983	3.20615409
6	1.78425091	1.68473397	2.59709928
6	1.17377604	3.03892439	2.96536536
1	0.95936703	-3.62228067	0.36939892
1	2.59074138	-2.94469289	0.55653182
1	0.93277776	-2.90140380	-2.01876183
1	2.22834494	-4.03965276	-1.64863925
1	3.94206974	-2.22654110	-1.83665396
1	1.60280613	-0.87884588	-3.31516424
1	3.30467263	-0.37229706	-3.33884099
1	2.27321003	0.00854322	-1.95703210
1	-2.88976550	-1.73094261	-0.42492460
1	-2.48119009	-1.50529853	-2.13602777
1	-2.92802922	0.74643943	-0.10831167
1	-4.10144526	0.19816246	-1.29469026
1	-2.54827897	0.86055726	-3.14714881
1	-1.36645573	1.40158236	-1.97051496
1	-4.17998884	2.59971903	-2.31148914

1 -2.67131603 3.34092819 -2.85470869

1 -2.98578496 3.14079251 -1.12876837

1 -0.81259290 -0.61186548 3.20638277

1 -0.99604816 1.13265600 2.96213184

1 1.63709585 -0.43284082 2.99971774

1 1.02626607 0.57773986 4.29899973

1 1.80976578 1.57722344 1.50854618

1 2.82761377 1.66029537 2.92977329

1 1.13029554 3.17412825 4.05110790

1 0.15807743 3.15047871 2.57621405

1 1.76864993 3.85885303 2.55381751

$end

Energy = -1115.5902114015

R4-A

$molecule

mult=2

cartesian

set=L1a_3

15 1.08046594 0.56300692 -0.94720920

8 2.06841366 0.85805978 -2.01241169

8 1.19754020 1.45048894 0.37958087

8 -0.45779721 0.74671743 -1.34951525

8 1.09597547 -0.92407172 -0.35875400

6	1.54050898	2.85869172	0.30085946
6	0.32448004	3.76726698	0.41140664
6	-0.36752103	3.78574028	1.78185493
6	-1.15317862	2.57052099	2.12602165
6	-0.92494467	0.39221668	-2.67992598
6	-1.52218991	-1.00495115	-2.71854581
6	-2.73690842	-1.19450927	-1.80783675
6	-3.32805705	-2.60214223	-1.89234974
6	2.35779834	-1.59191172	-0.07805542
6	2.66609159	-1.64922007	1.41136852
6	1.80785652	-2.61242161	2.24308667
6	0.34660305	-2.19773174	2.43492711
1	2.07752860	3.03806332	-0.63348344
1	2.22828422	3.02927408	1.13279986
1	-0.39746027	3.50494835	-0.36888702
1	0.67608635	4.78036353	0.18056948
1	-1.03203395	4.66727557	1.80895253
1	0.37846678	3.98553520	2.56560201
1	-1.50509754	2.41977941	3.13966925
1	-1.46746620	1.86882409	1.36463551
1	-0.09546055	0.49264507	-3.38327311
1	-1.67930170	1.14528142	-2.91958177
1	-0.74730198	-1.73678178	-2.46580292

1 -1.80655185 -1.20229834 -3.76072741

1 -3.50488577 -0.45778309 -2.07457945

1 -2.45087561 -0.97870081 -0.77418317

1 -4.19336676 -2.70971815 -1.23283310

1 -2.59199111 -3.35708546 -1.59935717

1 -3.65446223 -2.83749516 -2.91033439

1 3.15437448 -1.08181442 -0.62473360

1 2.24870001 -2.59669302 -0.49408875

1 2.60965419 -0.63726949 1.82672371

1 3.71575238 -1.95906565 1.49339878

1 2.27770048 -2.71433377 3.22787193

1 1.85042062 -3.60989168 1.78743810

1 -0.19876802 -2.17902876 1.49023687

1 0.27715602 -1.19694480 2.87156134

1 -0.16423746 -2.89283583 3.10790392

$end

Energy = -1115.5811693710

R4-B

$molecule

mult=2

cartesian

set=L1a_3

15 -0.49558081 -0.33827408 1.20712368

8	-0.95053491	-1.32330673	2.21693475
8	1.08778311	-0.20619040	1.02588545
8	-0.97842707	-0.58573538	-0.30031753
8	-0.95909795	1.17462538	1.44348562
6	1.96079292	-1.34835935	1.22836150
6	2.35454415	-2.02954885	-0.07421021
6	3.26826315	-1.21712733	-1.00186730
6	2.62653459	-0.08121927	-1.71711188
6	-2.38510549	-0.83492377	-0.55909787
6	-2.56427868	-1.12321813	-2.03798265
6	-1.87277635	-2.39954073	-2.52167480
6	-2.12179694	-2.68192261	-4.00378840
6	-1.07261825	1.71952594	2.78646271
6	0.13397854	2.55513837	3.18978663
6	0.29509567	3.90357721	2.47401728
6	0.72563642	3.82536301	1.00674528
1	1.46436221	-2.05219983	1.89992552
1	2.84030672	-0.94337539	1.73482873
1	1.45057768	-2.33598233	-0.61061486
1	2.87300610	-2.95362344	0.20956367
1	3.70333557	-1.91024953	-1.74162354
1	4.13816382	-0.85750545	-0.42915993
1	3.23069624	0.58515911	-2.32158844

1 1.55735990 0.07839920 -1.68793766

1 -2.95385502 0.05238156 -0.26619159

1 -2.70778773 -1.68071991 0.05472728

1 -2.20673919 -0.26163437 -2.61318970

1 -3.64354736 -1.19546537 -2.22324855

1 -2.22227396 -3.24837589 -1.92166616

1 -0.79677448 -2.31788319 -2.34208351

1 -3.18953392 -2.80203644 -4.21262502

1 -1.61599939 -3.59666415 -4.32403555

1 -1.75334198 -1.86297429 -4.62926888

1 -1.22724453 0.89347925 3.48431446

1 -1.97905823 2.32978893 2.76648663

1 1.04296538 1.95473462 3.07305239

1 0.02509642 2.74141830 4.26591992

1 1.03686404 4.49025786 3.02769181

1 -0.64637853 4.46200632 2.55266168

1 0.89469966 4.82805897 0.60292051

1 -0.02463802 3.33263374 0.38678249

1 1.65732649 3.26150845 0.90160603

$end

Energy = -1115.5820467601

R4-C

$molecule

mult=2

cartesian

set=L1a_3

15	0.53191693	0.22897901	1.35377213
8	0.92709540	0.49813030	2.75702630
8	1.71653463	0.24049086	0.27824068
8	-0.16257359	-1.18621238	1.07761471
8	-0.52033624	1.24938908	0.71155009
6	3.03181715	-0.27899768	0.61235422
6	3.18574427	-1.73400806	0.19685493
6	3.01920768	-1.97978974	-1.31094886
6	4.08744919	-1.37493139	-2.15048037
6	-1.10672107	-1.74655979	2.03057571
6	-2.54603480	-1.50170203	1.60803738
6	-2.92147403	-2.12877715	0.26385060
6	-4.38109028	-1.88180325	-0.11898685
6	-0.43702558	2.67334701	0.99656366
6	0.21056196	3.46356923	-0.13174075
6	-0.61455641	3.60828731	-1.41800949
6	-0.76072226	2.33523015	-2.25589814
1	3.20068671	-0.15290911	1.68407634
1	3.72883664	0.36047367	0.06735787
1	2.46779898	-2.34543172	0.75130962

1	4.18516875	-2.05784105	0.51436706
1	2.03643940	-1.62370621	-1.63686042
1	2.99753377	-3.07212492	-1.47095763
1	3.89844034	-1.09299591	-3.17912630
1	5.11268415	-1.33453201	-1.79760029
1	-0.90253963	-1.32976141	3.01932413
1	-0.88230270	-2.81572204	2.05167646
1	-2.73650369	-0.42329906	1.58361883
1	-3.18685807	-1.91229325	2.39967529
1	-2.73092527	-3.20850764	0.30504035
1	-2.26544295	-1.73123601	-0.51623676
1	-4.59144205	-0.81096376	-0.20060480
1	-5.06533303	-2.29621108	0.62822185
1	-4.62256934	-2.34105734	-1.08132317
1	0.10794180	2.80988760	1.93345792
1	-1.47106257	2.99149222	1.15141185
1	1.19041097	3.02928693	-0.35799648
1	0.40374767	4.46524846	0.27307714
1	-0.14287165	4.38261362	-2.03351934
1	-1.60865101	3.99570645	-1.16102444
1	0.21884422	1.92171160	-2.51374833
1	-1.28941526	2.54896215	-3.18961925
1	-1.31240914	1.55856832	-1.72437344

$end

Energy = -1115.5833581370

Table S2. Calculated molecular geometries and of TBP R1-R4 radicals at the DFT(B3LYP)/gen level of theory

R1

P	-0.560804482	-3.571541779	-1.973524703
O	0.121320696	-2.755537557	-3.167282413
O	0.004074032	-3.37658923	-0.614802647
O	-0.473812159	-5.08378378	-2.54932795
O	-2.109229563	-3.225098643	-2.168793888
C	0.341859664	-1.317931178	-3.033489503
H	-0.634100602	-0.820982399	-3.021637335
H	0.847682209	-1.128565402	-2.081550057
C	1.183245148	-0.86097793	-4.212975818
H	0.661062834	-1.118729824	-5.143441908
H	2.12933203	-1.417564476	-4.210268678
C	1.462831281	0.647854285	-4.170530576
H	0.5104679	1.19533097	-4.159773249
H	1.973437173	0.898055648	-3.230554942
C	2.31134937	1.121806298	-5.354834949
H	1.810620524	0.914224738	-6.308223063

H	2.496104907	2.200442852	-5.301342589
H	3.284029712	0.61547615	-5.372089676
C	0.536204475	-5.964731266	-2.152241991
H	1.328063424	-5.535178297	-1.545762177
C	0.74975896	-7.119196581	-3.064951438
H	1.174289325	-6.775309912	-4.027099885
C	1.677237432	-8.181986591	-2.454514991
H	2.635415969	-7.71537986	-2.188304013
C	1.926717316	-9.359534163	-3.401055017
H	2.393891007	-9.024737068	-4.33524077
H	2.589815543	-10.10127127	-2.942178197
H	0.988210384	-9.864373797	-3.660637627
C	-3.094998905	-3.708996607	-1.204948633
H	-3.150493388	-4.798425895	-1.296771439
H	-2.750702741	-3.453118282	-0.197799009
C	-4.433110698	-3.06113983	-1.518569862
H	-4.718605038	-3.316090965	-2.547818345
H	-5.178035839	-3.531203041	-0.86179559
C	-4.456319232	-1.539848246	-1.324228663
H	-3.69730595	-1.08068447	-1.969478194
H	-4.167762649	-1.305496234	-0.289971364

C	-5.827383969	-0.92756893	-1.626989374
H	-5.817720613	0.158345928	-1.48049865
H	-6.127368241	-1.122103931	-2.664043985
H	-6.602190837	-1.346664544	-0.973180834
H	1.23915625	-8.545412624	-1.516019594
H	-0.222879098	-7.567784636	-3.315417547

R2

P	-0.321187267	-3.464955523	-2.086493979
O	0.032856465	-2.652593355	-3.423060023
O	0.472013493	-3.11431374	-0.878645703
O	-0.218233228	-4.987665976	-2.581184511
O	-1.907011837	-3.256363536	-1.977681564
C	0.219873676	-1.208584509	-3.370393951
H	-0.745250487	-0.743867756	-3.13964681
H	0.924562918	-0.973752315	-2.566393731
C	0.742946402	-0.752136284	-4.722172994
H	0.029828725	-1.0545969	-5.500026833
H	1.686081117	-1.273646121	-4.931308261
C	0.961114106	0.766291276	-4.775289383
H	0.015349796	1.278780024	-4.551974574

H	1.66588499	1.061632575	-3.98596693
C	1.488833166	1.237589895	-6.134168083
H	0.788468324	0.984942847	-6.939458394
H	1.635423437	2.32335772	-6.146143489
H	2.450979459	0.76678601	-6.369626905
C	1.100889508	-5.621570226	-2.679345632
H	1.713554843	-4.998906304	-3.350508192
H	1.571091629	-5.61604878	-1.69011164
C	0.925006833	-7.000034866	-3.198159435
H	0.290733002	-7.12327618	-4.074321924
C	1.795758831	-8.13291649	-2.762391655
H	2.76682198	-8.091105215	-3.290575996
C	1.166213734	-9.511811163	-3.010784142
H	0.937157991	-9.652276186	-4.073666825
H	1.847634858	-10.31301545	-2.705185997
H	0.232581493	-9.625198231	-2.448674225
C	-2.626108027	-3.744428751	-0.806298878
H	-2.601307231	-4.838931785	-0.823409139
H	-2.109691882	-3.391860391	0.092547417
C	-4.054094407	-3.227563493	-0.865839497
H	-4.520126525	-3.578138929	-1.796415455

H	-4.603102458	-3.704559205	-0.042165044
C	-4.17602742	-1.702574045	-0.756071717
H	-3.609979948	-1.234776148	-1.570955826
H	-3.704531416	-1.370985607	0.1797302
C	-5.629961101	-1.222165279	-0.797572366
H	-5.689728115	-0.130929337	-0.717106286
H	-6.116864825	-1.515072025	-1.735925477
H	-6.213230643	-1.650949578	0.026712044
H	2.045375422	-8.019074402	-1.697444359

R3

P	-0.369765578	-3.515741611	-2.066930637
O	0.040019273	-2.698983537	-3.38418743
O	0.392117805	-3.192725071	-0.831848955
O	-0.279833276	-5.034512995	-2.575355394
O	-1.953681511	-3.280352496	-2.003843349
C	0.240551465	-1.257382728	-3.312585004
H	-0.725633149	-0.784339355	-3.104508081
H	0.924864046	-1.038018829	-2.48694565
C	0.806529367	-0.792631403	-4.64404241
H	0.110386892	-1.07430605	-5.444729404

H	1.74731977	-1.325381631	-4.834472285
C	1.048351767	0.722912964	-4.670284044
H	0.105086207	1.246629729	-4.462962031
H	1.737523034	0.996331968	-3.859569948
C	1.61688541	1.205354207	-6.008643943
H	0.932993297	0.97554695	-6.834662897
H	1.78047231	2.288727848	-6.000822175
H	2.577217301	0.7228687	-6.227262791
C	1.01309483	-5.698190156	-2.649846569
H	1.60035119	-5.224098126	-3.443943636
H	1.53585123	-5.569016788	-1.697798674
C	0.768726843	-7.171297579	-2.954370085
H	0.133719723	-7.23048809	-3.8579168
H	0.177325326	-7.614607729	-2.141626929
C	2.045889346	-7.926797776	-3.144632886
H	2.851540316	-7.437283621	-3.689678011
C	2.11632022	-9.403512023	-2.94231551
H	1.647903955	-9.959704076	-3.774999271
H	3.152194719	-9.753905752	-2.872604687
H	1.586325061	-9.712809324	-2.03117111
C	-2.716368072	-3.760457077	-0.856643924

H	-2.72311438	-4.854900643	-0.88738115
H	-2.212470689	-3.434170503	0.059016453
C	-4.126549875	-3.200743187	-0.945066979
H	-4.578821155	-3.525385552	-1.8916908
H	-4.71003904	-3.671867475	-0.141990039
C	-4.206577325	-1.674369499	-0.817405678
H	-3.607168772	-1.21281858	-1.61176074
H	-3.748921119	-1.369053683	0.134064893
C	-5.644390837	-1.150756522	-0.887661608
H	-5.674211117	-0.059373528	-0.793709184
H	-6.116331368	-1.416912117	-1.841496005
H	-6.26010155	-1.572775326	-0.083736713

R4

P	-0.39813538	-3.495275332	-2.036433268
O	-0.007428289	-2.706319729	-3.376223192
O	0.378559082	-3.143483986	-0.818505703
O	-0.310118843	-5.02463281	-2.512395479
O	-1.981842201	-3.262367435	-1.958561776
C	0.19060996	-1.26316157	-3.340311327
H	-0.776167226	-0.787243187	-3.141729658

H	0.87629013	-1.022139085	-2.52188632
C	0.753020397	-0.830719571	-4.684123732
H	0.056818976	-1.135660712	-5.476196728
H	1.695421129	-1.364973647	-4.862022049
C	0.989363766	0.684491511	-4.750400581
H	0.044274181	1.210109541	-4.556629173
H	1.677811922	0.98177162	-3.94750493
C	1.555676666	1.133365696	-6.101312113
H	0.872420314	0.879132462	-6.920672385
H	1.715175762	2.21717594	-6.122323691
H	2.517773867	0.64889906	-6.30743221
C	0.983606402	-5.68906942	-2.57809234
H	1.574593019	-5.218370857	-3.371716093
C	0.740860502	-7.160476999	-2.870301954
H	0.179913832	-7.25021887	-3.809164959
C	2.057477661	-7.950315454	-2.974542481
H	2.695498158	-7.46942627	-3.740897287
C	1.852348714	-9.389876303	-3.309620877
H	1.038887462	-9.694459673	-3.96238708
H	2.604235215	-10.13128123	-3.05830633
C	-2.729368631	-3.724808897	-0.794249804

H	-2.736368717	-4.81958101	-0.808452666
H	-2.213504585	-3.384820412	0.109705372
C	-4.140503236	-3.165948241	-0.87235233
H	-4.604992775	-3.503663846	-1.808431585
H	-4.713714533	-3.625479464	-0.055278586
C	-4.21835923	-1.637891182	-0.7651145
H	-3.628728538	-1.187898733	-1.573284118
H	-3.748651629	-1.319591164	0.176176562
C	-5.656679839	-1.114381165	-0.824683585
H	-5.684797721	-0.021764038	-0.745720666
H	-6.14066865	-1.393602313	-1.768692636
H	-6.262448333	-1.524660576	-0.007247577
H	2.622233317	-7.861124858	-2.035439704
H	0.113345172	-7.584542774	-2.077261206
H	1.50120902	-5.54894357	-1.623708894

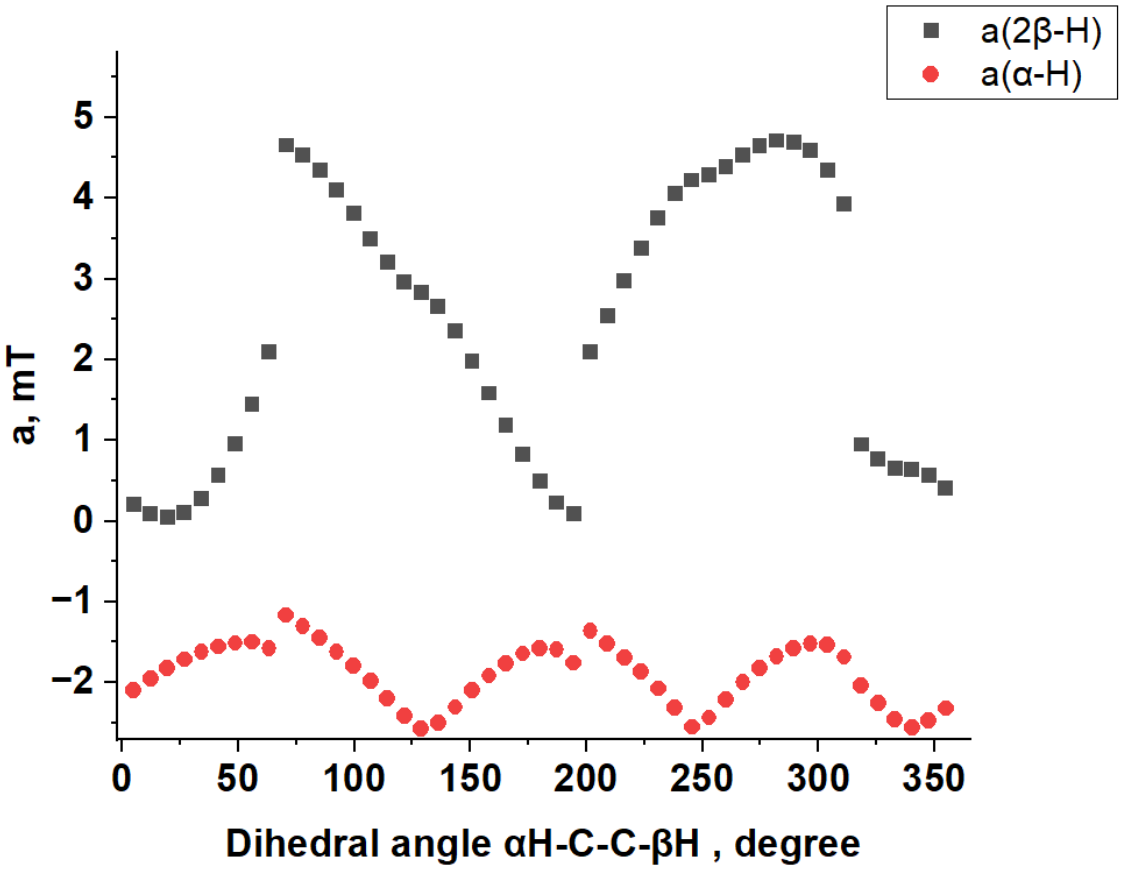

Figure S1. The HFC constants for alpha and beta-protons of radical R1 calculated at the DFT(B3LYP)/L1a_3 level of theory as a function of dihedral angle αH-C-C-βH.

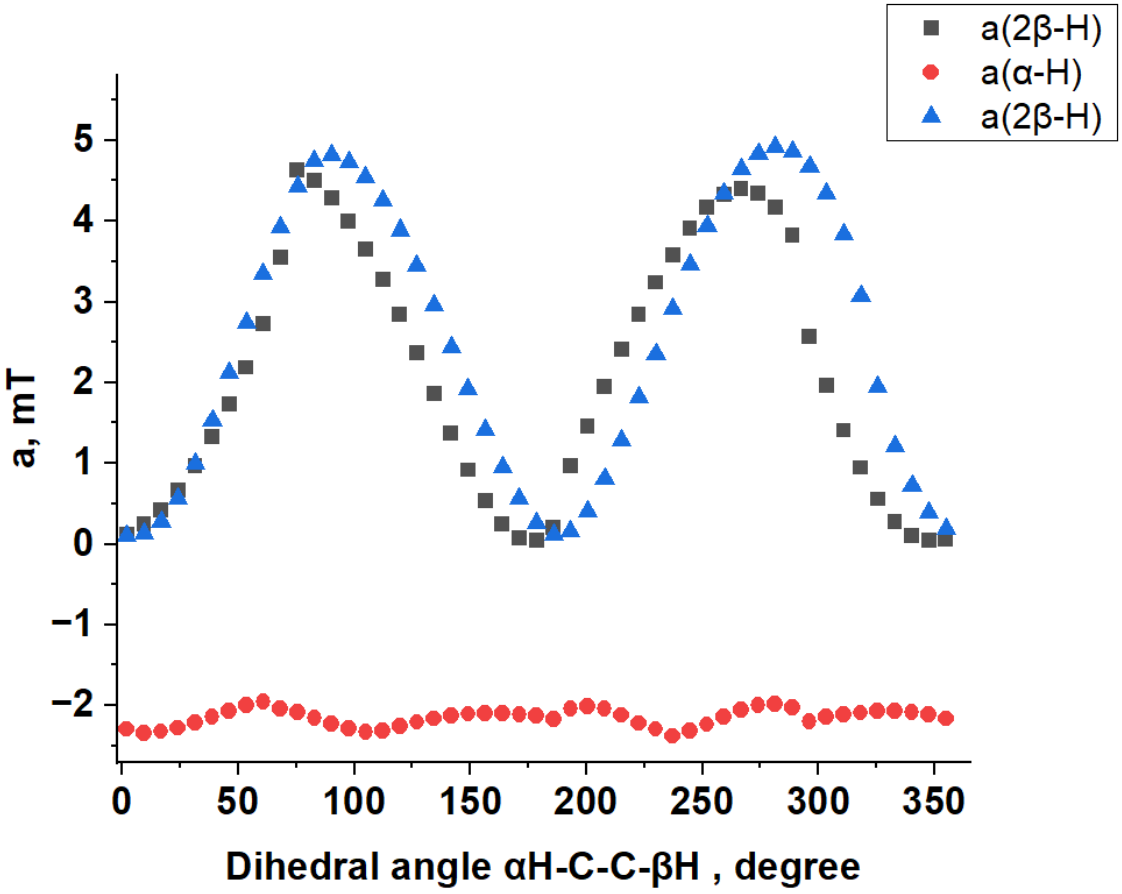

Figure S2. The HFC constants for alpha and beta-protons of radical R2 calculated at the DFT(B3LYP)/L1a_3 level of theory as a function of dihedral angle αH-C-C-βH.

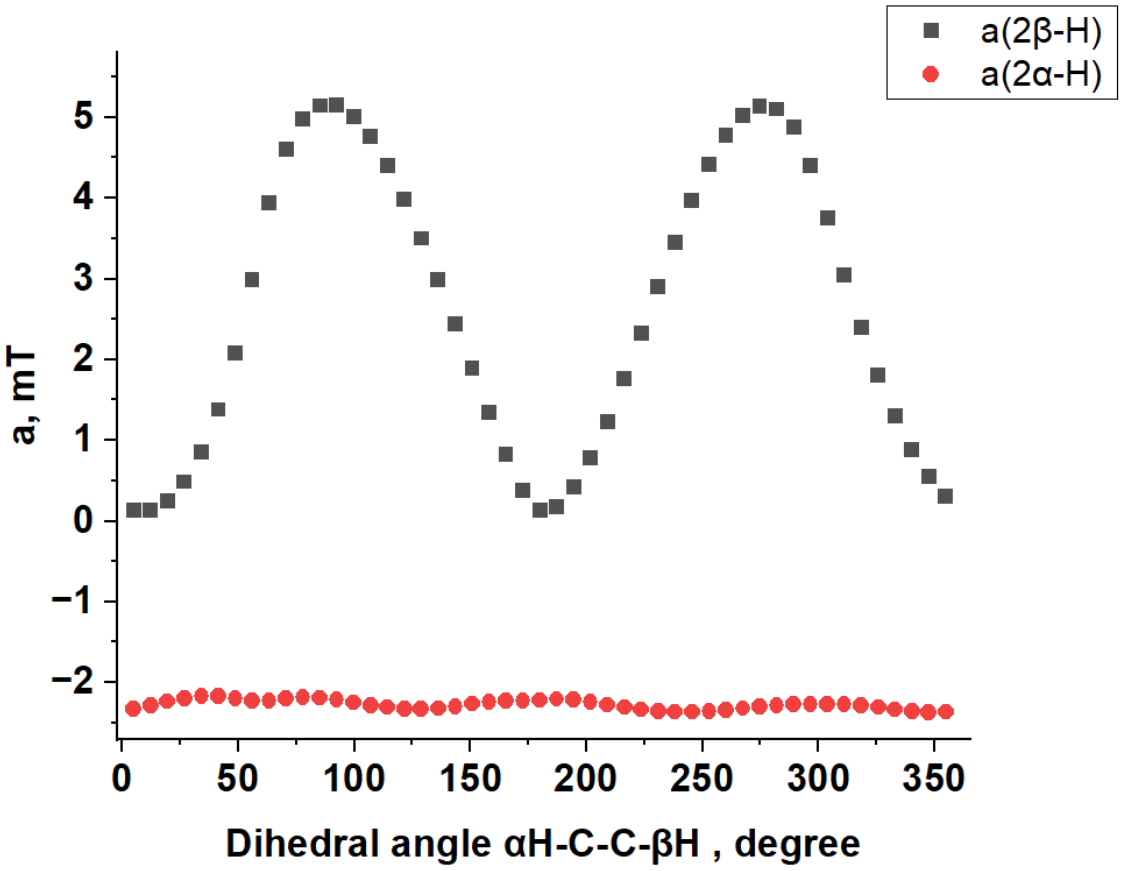

Figure S3. The HFC constants for alpha and beta-protons of radical R4 calculated at the DFT(B3LYP)/L1a_3 level of theory as a function of dihedral angle αH-C-C-βH.