Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Thermal Denitrogenation of 7-Isopropylidene-2,3-diaza-norbornene: Formation of Substituted 3-Methylene-(1,4)-pentadienes

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1 Supporting Information

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Table S1: Electronic energies (in a.u.) and ZPVEs (in kcal mol^{-1}) at optimized CASSCF/6-311G(d,p) geometries.

Structure	**CASSCF**	**MRMP2**[a]	**MRMP2**[b]	**ZPVE**
1	−309.939568[c]	−311.053281	−311.055738	114.4
21	−309.943626[c]	−311.058143	−311.058226	114.2
5/6	−309.948617[d]	−311.041675	−-311.04066	111.4

[a] Singlet
[b] Vertical triplet
[c] Active space: (4*e*,4*o*)
[d] Active space: (6*e*,6*o*)

Table S2: Electronic energies (in a.u.) and ZPVEs (in kcal mol^{-1}) of minima at optimized B3LYP/6-311G(d,p) geometries.

Structure	**B3LYP**	**CCSD(T)**	**ZPVE**
1		−311.166766[a]	107.5
2	−421.609002	−420.488504	118.5
3	−312.067484	−311.189208	110.2
4	−312.103108	−311.219952	109.0
5	−312.103696	−311.221536	109.0
6	−312.103014	−311.220551	108.8
7	−312.132071	−311.254365	111.4
9	−312.082379	−311.200508	108.9
10	−312.055943	−311.184232	110.5
11	−312.094583	−311.218672	109.7
12	−312.038898	−311.170019	110.2
13	−312.097447	−311.218658	109.9
14	−312.101729	−311.221006	109.7
15	−312.043442	−311.170590	110.3
16	−312.038565	−311.168628	110.3
17	−312.006341	−311.126403	107.5
18	−312.080324	−311.200147	108.5
19	−312.071193	−311.196478	109.1
20	−312.084875	−311.201362	108.6
21		−311.168272[a]	107.5
22	−312.132120	−311.252979	110.0
23	−312.136399	−311.257882	110.6

[a] Energy of vertical triplet at optimized CASSCF geometry

Table S3: Electronic energies (in a.u.) and ZPVEs (in kcal mol^{-1}) of TSs at optimized B3LYP/6-311G(d,p) geometries.

Structure	**B3LYP**	**CCSD(T)**	**ZPVE**
1/2	−421.569855	−420.443793	115.4
1/3	−312.038596	−311.159028	107.9
1/4	−312.017866	−311.132129	106.7
1/7	−312.011736	−311.129550	106.3
1/12	−312.031220	−311.153415	108.3
4/6	−312.047780	−311.160142	106.8
4/11	−312.035660	−311.154986	107.8
5/13	−312.032931	−311.152136	108.1
5/14	−312.035899	−311.153601	107.9
6/13	−312.041556	−311.159604	108.1
6/14	−312.045150	−311.161571	107.7
9/18	−312.018418	−311.139701	107.7
11/12	−312.001671	−311.128553	108.5
13/15	−312.006705	−311.129653	108.5
14/16	−312.004293	−311.129238	108.7
18/19	−312.011478	−311.133071	105.8
19/20	−312.009558	−311.129159	105.8
20/21	−312.020469	−311.141594	107.3
21/22	−312.017965	−311.133400	105.6
21/23	−312.019793	−311.134787	105.7

Table S4: Optimized geometry of **1** at (4*e*,4*o*)CASSCF/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−0.009123	0.019128	0.024393
C	0.949596	1.064948	0.031059
C	0.688386	−1.216090	0.030459
C	2.355630	0.526455	0.082960
C	2.180401	−1.011331	0.010827
C	−1.420607	0.164909	0.016079
H	2.855558	0.826915	1.001409
H	2.962355	0.904561	−0.736076
H	2.667318	−1.514859	0.842162
H	2.618942	−1.419752	−0.897228
H	0.731004	2.113548	0.054630
H	0.233679	−2.185983	−0.005446
C	−2.101971	1.502174	−0.092518
C	−2.330462	−1.036983	0.002271
H	−1.408392	2.329066	−0.159822
H	−2.746460	1.676291	0.767869
H	−2.739886	1.533606	−0.975101
H	−1.937202	−1.859021	0.589005
H	−2.490203	−1.402272	−1.012320
H	−3.305169	−0.781357	0.407455

Table S5: Optimized geometry of **2** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−0.324074	−0.000011	−0.081622
C	0.709856	−1.101901	−0.133676
C	1.571658	−0.778930	1.128290
C	0.709866	1.101864	−0.133933
C	1.571452	0.779268	1.128251
C	−1.653234	−0.000001	−0.007797
C	−2.465193	−1.270852	0.039011
C	−2.465196	1.270859	0.038703
N	1.575911	−0.623132	−1.269164
N	1.576193	0.622761	−1.269089
H	0.418292	−2.138967	−0.264559
H	2.571457	−1.207218	1.041113
H	1.096423	−1.188272	2.021266
H	0.418311	2.138890	−0.265154
H	1.095918	1.188563	2.021088
H	2.571156	1.207814	1.041236
H	−3.183275	−1.295967	−0.788338
H	−1.849071	−2.167785	−0.020357
H	−3.051196	−1.320798	0.963998
H	−3.182945	1.295993	−0.788936
H	−3.051571	1.320793	0.963453
H	−1.849041	2.167785	−0.020403

Table S6: Optimized geometry of **3** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.046376	−0.791364	0.627804
C	2.130378	−0.781201	−0.466825
C	1.046352	0.791152	0.627964
C	2.130033	0.781404	−0.466939
C	−0.114403	−0.000050	0.228915
C	−1.418578	−0.000013	−0.016655
C	−2.198903	−1.281965	−0.160255
C	−2.198868	1.281978	−0.160110
H	1.032245	−1.468173	1.475862
H	1.860210	−1.277057	−1.402746
H	3.081699	−1.186286	−0.117618
H	1.032308	1.467784	1.476165
H	3.081216	1.186892	−0.117844
H	1.859540	1.277104	−1.402863
H	−2.707098	−1.323969	−1.131037
H	−1.552768	−2.156796	−0.071939
H	−2.980968	−1.354996	0.605495
H	−2.707258	1.324045	−1.130788
H	−2.980774	1.355015	0.605801
H	−1.552677	2.156778	−0.071883

Table S7: Optimized geometry of **4** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.255709	−0.000016	0.000093
C	−0.104054	−0.000012	−0.000006
C	−0.854909	−1.263120	0.178859
C	−2.066286	−1.556924	−0.302584
C	−0.854827	1.263127	−0.178951
C	−2.066297	1.556943	0.302251
H	−0.352915	−2.032312	0.757356
H	−2.513598	−2.526422	−0.114954
H	−0.352665	2.032348	−0.757266
H	−2.513530	2.526471	0.114596
H	−2.639830	0.859549	0.900368
H	−2.639661	−0.859553	−0.900876
C	2.093525	1.252780	−0.079535
H	2.891665	1.210771	0.670500
H	2.592417	1.330052	−1.054076
H	1.532712	2.169143	0.092635
C	2.093553	−1.252791	0.079835
H	2.592268	−1.330080	1.054466
H	1.532817	−2.169170	−0.092482
H	2.891836	−1.210719	−0.670045

Table S8: Optimized geometry of **5** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−1.416824	−0.194632	−0.023405
C	0.075709	−0.110380	−0.086318
C	0.622457	1.166039	−0.601167
C	1.625759	1.872135	−0.076791
C	0.827025	−1.163373	0.287651
C	2.316831	−1.318126	0.208572
C	−2.081873	−1.223246	−0.558292
C	−2.131616	0.941099	0.670721
H	0.115988	1.563542	−1.480229
H	1.955890	2.800266	−0.530081
H	2.136366	1.559066	0.826923
H	0.291199	−2.025843	0.676652
H	2.569435	−2.297545	−0.211788
H	2.785850	−0.545520	−0.401322
H	2.774888	−1.283452	1.204586
H	−3.162498	−1.293816	−0.490013
H	−1.567080	−2.017407	−1.086153
H	−3.212434	0.788838	0.669981
H	−1.793118	1.034756	1.708189
H	−1.919305	1.900021	0.187426

Table S9: Optimized geometry of **6** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	0.973907	−0.620898	0.178731
C	−0.346469	0.043475	−0.075824
C	−1.510789	−0.866536	−0.139026
C	−2.745789	−0.591979	0.286480
C	−0.474074	1.367267	−0.270879
C	0.607084	2.404443	−0.229693
C	1.590413	−0.512994	1.356647
C	1.553536	−1.419622	−0.964697
H	−1.314366	−1.860921	−0.534705
H	−3.545037	−1.318274	0.194499
H	−2.995569	0.357165	0.748482
H	−1.468509	1.738278	−0.509724
H	0.624895	2.981494	−1.161248
H	0.421677	3.125248	0.575869
H	1.593572	1.969726	−0.067363
H	2.543138	−0.998380	1.543498
H	1.158214	0.057133	2.171001
H	2.486077	−1.908446	−0.675990
H	0.858127	−2.191602	−1.310238
H	1.750865	−0.770359	−1.824512

Table S10: Optimized geometry of **7** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	0.048115	0.003286	−0.017238
C	−0.662678	−1.137114	−0.036689
C	−2.148285	−0.901504	−0.116576
C	−0.881208	1.206512	−0.079665
C	−2.279362	0.607880	0.204207
C	1.510996	0.113358	0.005478
C	2.314692	−1.164192	0.078527
C	2.125068	1.305524	−0.043941
H	−0.235054	−2.132662	−0.039168
H	−2.718822	−1.530471	0.574686
H	−2.520030	−1.137859	−1.123498
H	−0.829458	1.669111	−1.073590
H	−0.612071	1.983425	0.641373
H	−3.072424	1.095863	−0.365956
H	−2.517629	0.731389	1.264137
H	3.384438	−0.951468	0.105334
H	2.058694	−1.741926	0.972286
H	2.116913	−1.805193	−0.786510
H	3.206555	1.380798	−0.032006
H	1.574862	2.236496	−0.101706

Table S11: Optimized geometry of **9** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.902489	0.022673	−0.042692
C	0.778388	−0.634160	−0.353495
C	−0.593471	−0.072635	−0.602337
C	−1.614351	−0.538915	0.467704
C	−2.969240	−0.058003	0.213045
C	−4.074777	0.353049	−0.017938
H	0.843012	−1.719173	−0.433600
H	−0.588581	1.018013	−0.630818
H	−0.954235	−0.406591	−1.581954
H	−1.621647	−1.634117	0.511395
H	−1.283733	−0.195270	1.453817
H	−5.055011	0.711117	−0.215489
C	3.197507	−0.722169	0.172717
H	3.072271	−1.799782	0.051576
H	3.965106	−0.386055	−0.534494
H	3.595252	−0.534475	1.177023
C	2.012752	1.518301	0.115698
H	1.066020	2.039767	−0.020615
H	2.395493	1.769513	1.111643
H	2.730275	1.928220	−0.604691

Table S12: Optimized geometry of **10** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	0.103933	−0.096060	−0.842330
C	0.124517	−0.798654	0.460555
C	1.434300	−0.313246	1.100103
C	1.271407	0.462397	−1.162183
C	2.327693	0.006399	−0.148411
C	−1.119155	0.023269	−0.022542
C	−2.340059	−0.820618	−0.349361
C	−1.451090	1.383629	0.560972
H	−0.070378	−1.869508	0.479501
H	1.873685	−1.061537	1.765169
H	1.286013	0.599738	1.687560
H	1.447676	1.238305	−1.899485
H	3.068243	0.788959	0.045495
H	2.884001	−0.880373	−0.481345
H	−2.057723	−1.790386	−0.763784
H	−2.941981	−0.988983	0.548951
H	−2.966894	−0.310576	−1.087503
H	−1.990507	1.996006	−0.168411
H	−2.091298	1.268942	1.442032
H	−0.550114	1.926704	0.851011

Table S13: Optimized geometry of **11** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	0.727968	−0.339562	0.000006
C	−0.412924	0.698245	−0.000030
C	1.686789	0.917309	−0.000248
C	0.425877	1.751022	−0.000153
C	−1.857393	0.594925	0.000091
C	−2.561137	−0.543765	−0.000111
H	2.320134	1.007462	−0.889392
H	2.320457	1.007620	0.888644
H	0.262658	2.823669	−0.000135
H	−2.392596	1.543226	0.000342
H	−3.644608	−0.536463	−0.000033
H	−2.080740	−1.515224	−0.000407
C	0.832479	−1.193465	−1.266639
H	1.788712	−1.726511	−1.293696
H	0.034410	−1.940262	−1.312181
H	0.761678	−0.574669	−2.165189
C	0.832514	−1.192942	1.267017
H	0.033096	−1.938203	1.313979
H	1.787787	−1.727755	1.293195
H	0.763975	−0.573484	2.165282

Table S14: Optimized geometry of **12** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	0.965692	0.050749	−0.000058
C	−0.404363	0.206157	−0.646144
C	0.110185	−0.750447	1.090927
C	−1.077972	−0.932226	0.074014
C	−1.469305	1.032414	−0.611852
C	−2.351476	−0.018796	0.080087
H	−0.153040	−0.107239	1.933195
H	0.570986	−1.672598	1.455106
H	−1.163440	−1.931292	−0.354693
H	−1.580177	2.106364	−0.715608
H	−2.662392	0.290175	1.083801
H	−3.225201	−0.410088	−0.451671
C	1.671647	1.318177	0.464862
H	2.511989	1.076151	1.123848
H	2.070269	1.878082	−0.387022
H	0.987110	1.973427	1.009330
C	1.915610	−0.881576	−0.758781
H	2.333333	−0.378143	−1.635453
H	2.747216	−1.188019	−0.116248
H	1.403235	−1.783534	−1.102918

Table S15: Optimized geometry of **13** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−0.040617	−0.310821	−0.114987
C	1.311968	0.353776	−0.392352
C	0.495067	−1.537994	0.038608
C	1.916717	−1.089528	−0.221689
C	−1.402303	0.206810	−0.066104
C	−1.673128	1.480543	−0.387058
C	−2.485723	−0.760663	0.345639
C	1.806866	1.404643	0.597875
H	1.405936	0.725486	−1.419004
H	0.070477	−2.512854	0.251930
H	2.391626	−1.501221	−1.118478
H	2.612912	−1.191195	0.617797
H	−2.685449	1.867864	−0.361119
H	−0.893805	2.168192	−0.692900
H	−3.465914	−0.281071	0.348001
H	−2.524643	−1.615999	−0.336763
H	−2.293934	−1.158818	1.347112
H	1.730568	1.035074	1.625037
H	2.854512	1.656250	0.404911
H	1.224617	2.327688	0.533883

Table S16: Optimized geometry of **14** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−0.108919	−0.352619	−0.091863
C	−0.318709	1.123218	−0.434825
C	1.236851	−0.243291	−0.018796
C	1.247931	1.235833	−0.354247
C	−1.024712	−1.461498	0.065902
C	−2.346229	−1.406616	−0.143628
C	2.357322	−1.184609	0.256143
C	−1.102763	1.982283	0.553964
H	−0.694495	1.281185	−1.452460
H	1.744259	1.507175	−1.292908
H	1.614769	1.900587	0.436409
H	−0.582108	−2.408129	0.371147
H	−2.976436	−2.278397	−0.014740
H	−2.836069	−0.491023	−0.456098
H	3.044615	−1.234543	−0.596669
H	2.948777	−0.850845	1.116840
H	1.999868	−2.196263	0.461979
H	−0.727250	1.841755	1.572245
H	−1.014309	3.044099	0.302803
H	−2.166254	1.728188	0.555553

Table S17: Optimized geometry of **15** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−1.240686	−0.578980	0.378174
C	0.020983	−0.259558	−0.409460
C	−1.096034	0.938735	0.838457
C	−0.124423	1.238931	−0.366751
C	1.359468	−0.268770	−0.225862
C	1.434144	1.270144	−0.221740
H	−0.602795	1.018578	1.809192
H	−2.027924	1.511134	0.849709
H	−0.573529	1.807124	−1.182838
H	1.776681	1.663680	0.742073
H	1.985558	1.779261	−1.020326
C	−2.506840	−0.865463	−0.425401
H	−2.470535	−1.864319	−0.868901
H	−3.392700	−0.811830	0.214923
H	−2.633098	−0.143990	−1.237894
H	−1.119597	−1.319547	1.174005
C	2.352051	−1.297276	0.197537
H	1.887622	−2.283593	0.279937
H	3.179891	−1.376693	−0.517182
H	2.798448	−1.046381	1.167573

Table S18: Optimized geometry of **16** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−1.295652	−0.658726	0.215947
C	0.031438	−0.710003	−0.519140
C	−0.456460	0.232438	1.236653
C	0.674221	0.484194	0.155064
C	1.138691	−1.478427	−0.507920
C	1.986103	−0.381412	0.152344
H	−0.111919	−0.352640	2.090991
H	−0.966891	1.134988	1.585250
H	2.317695	−0.669853	1.155900
H	2.840154	0.037645	−0.390819
C	−2.466382	0.056630	−0.453955
H	−2.885721	−0.557061	−1.256078
H	−3.262730	0.253507	0.270363
H	−2.162866	1.011013	−0.890651
H	−1.625571	−1.620170	0.618934
C	0.756523	1.883176	−0.426176
H	1.300100	2.550121	0.253332
H	1.287851	1.876080	−1.382624
H	−0.231434	2.319898	−0.595132
H	1.290440	−2.550744	−0.576369

Table S19: Optimized geometry of **17** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.849986	0.024440	0.018740
C	0.766089	−0.710577	0.297147
C	−0.601564	−0.236110	0.703864
C	−1.657187	−0.521663	−0.387379
C	−3.053631	−0.119245	0.038639
C	−3.877306	0.750266	−0.456574
C	3.147692	−0.635350	−0.378556
C	1.908575	1.530044	0.072865
H	0.863283	−1.792609	0.213664
H	−0.904836	−0.752517	1.623643
H	−0.611127	0.830877	0.932639
H	−1.392181	0.009456	−1.303794
H	−1.661452	−1.589606	−0.629268
H	−3.511381	−0.590920	0.920121
H	3.949069	−0.375427	0.323081
H	3.059797	−1.723008	−0.406950
H	3.475571	−0.292386	−1.366900
H	2.668751	1.858199	0.791209
H	2.206628	1.935258	−0.900898
H	0.961954	1.991844	0.350983

Table S20: Optimized geometry of **18** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−1.975901	−0.366769	−0.367850
C	−0.729411	−0.312568	−0.747391
C	0.439331	0.289783	0.040541
C	1.363767	−0.865277	0.394166
C	2.615863	−1.056497	−0.011354
C	−3.224995	−0.422524	0.003152
H	−0.462760	−0.743165	−1.711689
H	0.907882	−1.603942	1.051578
H	3.178035	−1.926161	0.310301
H	3.130766	−0.365810	−0.669270
H	−3.612896	−1.267516	0.564666
H	−3.924628	0.372590	−0.237678
C	−0.045827	0.946185	1.347010
H	−0.758996	1.747026	1.135469
H	−0.540844	0.220208	1.996310
H	0.801508	1.369944	1.891626
C	1.124464	1.345704	−0.845920
H	1.995123	1.773133	−0.341043
H	1.456587	0.919270	−1.796181
H	0.426477	2.156200	−1.068221

Table S21: Optimized geometry of **19** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−0.319586	−0.322643	−0.865948
C	0.901751	−0.247820	0.062309
C	0.346414	1.020074	−0.537433
C	−1.626259	−0.644677	−0.369185
C	−2.725911	−0.919824	0.036720
H	−0.122113	−0.712057	−1.860340
H	−3.696162	−1.167146	0.390650
C	−0.368606	2.089878	0.256585
H	−1.046902	1.669911	0.999672
H	0.348884	2.734252	0.774155
H	−0.965704	2.721315	−0.407758
H	0.932284	1.414698	−1.363737
C	0.726177	−0.542410	1.539585
H	0.820248	−1.617083	1.724046
H	1.499724	−0.034096	2.124673
H	−0.247499	−0.232354	1.917552
C	2.205787	−0.773847	−0.511304
H	3.062875	−0.313812	−0.007650
H	2.283580	−1.858037	−0.379786
H	2.292186	−0.557984	−1.579451

Table S22: Optimized geometry of **20** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−2.115456	−0.031511	−0.280601
C	−0.910897	0.344424	−0.609169
C	0.248514	0.531119	0.364916
C	1.362903	−0.459893	0.036134
C	2.529416	−0.098541	−0.499638
C	−3.318000	−0.406030	0.057677
H	−0.690364	0.557218	−1.654755
H	−0.125653	0.274960	1.363038
H	3.290792	−0.836487	−0.729125
H	2.774298	0.931739	−0.725892
H	−3.603571	−1.453828	0.071127
H	−4.079768	0.316809	0.334842
C	1.052736	−1.901302	0.354223
H	0.873878	−2.031414	1.427942
H	0.143606	−2.230973	−0.157922
H	1.872129	−2.560674	0.062830
C	0.682048	2.004289	0.383371
H	1.519556	2.157903	1.068540
H	0.987364	2.346067	−0.609519
H	−0.149855	2.633350	0.707409

Table S23: Optimized geometry of **21** at (4*e*,4*o*)CASSCF/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.511133	−0.032133	−0.012612
C	0.747447	1.070509	−0.370548
C	0.591096	−1.227409	0.201175
C	−0.730578	0.782208	−0.421049
C	−0.785299	−0.672200	−0.010129
C	2.885500	−0.078194	0.126568
H	0.724069	−1.670126	1.200619
H	0.827918	−2.038065	−0.509266
H	3.494637	0.801480	−0.045222
H	3.395511	−0.990761	0.410428
H	−1.106471	0.907129	−1.455147
H	1.163214	2.047742	−0.590865
C	−2.004185	−1.520986	−0.094190
H	−2.081062	−2.031367	−1.069975
H	−2.003475	−2.310168	0.666114
H	−2.921613	−0.938404	0.029673
C	−1.572063	1.730326	0.465116
H	−1.474272	2.766215	0.126348
H	−2.632728	1.466826	0.424944
H	−1.244037	1.676777	1.506363

Table S24: Optimized geometry of **21** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.511133	−0.032133	−0.012612
C	0.747447	1.070509	−0.370548
C	0.591096	−1.227409	0.201175
C	−0.730578	0.782208	−0.421049
C	−0.785299	−0.672200	−0.010129
C	2.885500	−0.078194	0.126568
H	0.724069	−1.670126	1.200619
H	0.827918	−2.038065	−0.509266
H	3.494637	0.801480	−0.045222
H	3.395511	−0.990761	0.410428
H	−1.106471	0.907129	−1.455147
H	1.163214	2.047742	−0.590865
C	−2.004185	−1.520986	−0.094190
H	−2.081062	−2.031367	−1.069975
H	−2.003475	−2.310168	0.666114
H	−2.921613	−0.938404	0.029673
C	−1.572063	1.730326	0.465116
H	−1.474272	2.766215	0.126348
H	−2.632728	1.466826	0.424944
H	−1.244037	1.676777	1.506363

Table S25: Optimized geometry of **22** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	1.562471	−0.000003	0.000444
C	0.668706	1.231483	0.001737
C	0.668713	−1.231477	0.001735
C	−0.738206	0.670326	0.000086
C	−0.738202	−0.670312	0.000124
C	2.891553	−0.000006	−0.002121
H	0.851428	1.868750	−0.874255
H	0.849972	1.865620	0.880381
H	0.850049	−1.865816	0.880196
H	0.851301	−1.868551	−0.874445
H	3.461384	0.923567	−0.003225
H	3.461365	−0.923591	−0.003184
C	−1.910821	−1.602412	−0.000877
H	−2.866812	−1.076851	−0.001792
H	−1.887323	−2.258471	−0.879319
H	−1.888816	−2.258362	0.877680
C	−1.910823	1.602393	−0.000888
H	−2.866796	1.076823	−0.001501
H	−1.888680	2.258615	0.877480
H	−1.887426	2.258309	−0.879457

Table S26: Optimized geometry of **23** at B3LYP/6-311G(d,p) level.

Atom	x (Å)	y (Å)	z (Å)
C	−1.547147	0.080085	−0.033533
C	−0.747511	−1.196108	0.193016
C	0.720374	−0.736369	0.416563
C	−0.574194	1.160228	−0.161401
C	0.682515	0.745369	0.069594
C	−2.878928	0.187819	−0.098956
H	−0.808121	−1.830536	−0.697939
H	−1.135730	−1.782113	1.029265
H	0.979054	−0.827207	1.481822
H	−0.856206	2.181881	−0.392044
H	−3.527678	−0.672497	0.022094
H	−3.358971	1.143909	−0.276543
C	1.918345	1.588095	0.062196
H	2.626106	1.256365	−0.705675
H	1.686179	2.638323	−0.124897
H	2.444648	1.519381	1.021929
C	1.747759	−1.551397	−0.381074
H	2.770415	−1.214784	−0.189949
H	1.694158	−2.609792	−0.110379
H	1.558867	−1.469266	−1.456115