Supplementary Data for

Mass-spectrometric and Computational Study of Tryptophan Radicals (Trp + H)$^{\bullet}$ Produced by Collisional Electron Transfer to Protonated Tryptophan in the Gas Phase

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Tables S1-S33 of B3LYP optimized geometries, B3LYP, MP2 and ROMP2 total, and zero-point energies. Table S34 with vertical excitation energies.

Table S1. B3LYP/6-31+G(d,p) optimized structure of **1**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.364598	-0.838595	1.210502
2	1	0	-1.762916	-1.737820	0.889763
3	1	0	-1.527548	-0.778877	2.219320
4	1	0	-0.343038	-0.809789	1.038534
5	6	0	-2.062284	0.268898	0.447832
6	1	0	-2.188049	1.113689	1.127933
7	6	0	-1.207162	0.705394	-0.778877
8	6	0	-3.417868	-0.307933	0.042549
9	1	0	-1.258556	-0.076629	-1.546319
10	1	0	-1.696977	1.588815	-1.197624
11	6	0	0.218167	0.984241	-0.405762
12	8	0	-3.658062	-1.496812	0.112322
13	6	0	0.763180	2.192247	-0.020632
14	6	0	1.283731	0.006304	-0.327186
15	1	0	0.305898	3.170981	0.033007
16	7	0	2.088162	2.020532	0.298481
17	6	0	2.443268	0.696302	0.125962
18	6	0	1.382831	-1.373400	-0.619790
19	1	0	2.716471	2.762187	0.570994
20	6	0	3.672134	0.053066	0.312991
21	6	0	2.602569	-2.014213	-0.430900
22	1	0	0.542060	-1.925330	-1.035940
23	1	0	4.548946	0.594637	0.654337
24	6	0	3.732708	-1.308299	0.035709
25	1	0	2.695710	-3.069902	-0.664403
26	1	0	4.671345	-1.836527	0.166710
27	8	0	-4.236739	0.632544	-0.413598
28	1	0	-5.077524	0.229507	-0.700360

Rotational constants (GHZ): 1.3031023 0.3394473 0.2879143
E[B3LYP/6-31+G(d,p)] = -686.79104551 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.95347053 a.u.
E[PMP2/6-311++G(2d,p)] = -685.15321183 a.u.
ZPVE = 612.8129 kJ mol^{-1}

Table S2. B3LYP/6-31+G(d,p) optimized structure of **2**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.003392	1.045656	-1.027246
2	1	0	-3.345778	1.136761	-1.979478
3	1	0	-3.752356	1.314109	-0.392573
4	6	0	-2.575423	-0.322679	-0.751878
5	1	0	-3.214074	-1.083784	-1.229879
6	6	0	-1.138455	-0.579252	-1.267890

7	6	0	-2.700577	-0.587672	0.748018
8	1	0	-0.893785	-1.635057	-1.127043
9	1	0	-1.126779	-0.397565	-2.350307
10	6	0	-0.071919	0.268149	-0.628060
11	8	0	-3.240858	0.158122	1.533780
12	6	0	-0.196561	1.538498	-0.204140
13	6	0	1.309040	-0.186483	-0.372612
14	1	0	-1.035900	2.217267	-0.223611
15	7	0	1.101296	2.004573	0.381504
16	6	0	2.023292	0.849397	0.233958
17	6	0	1.966899	-1.393069	-0.618595
18	1	0	0.981627	2.272979	1.367011
19	6	0	3.347517	0.775119	0.619866
20	6	0	3.311179	-1.505587	-0.244440
21	1	0	1.455372	-2.226673	-1.087587
22	1	0	3.871771	1.600151	1.092275
23	6	0	3.992967	-0.444233	0.364118
24	1	0	3.837775	-2.436072	-0.429446
25	1	0	5.034378	-0.561509	0.643711
26	8	0	-2.161160	-1.775493	1.096030
27	1	0	-2.338696	-1.922127	2.041893
28	1	0	1.449497	2.835751	-0.113321

Rotational constants (GHZ): 0.9601849 0.4666515 0.3647595

E[B3LYP/6-31+G(d,p)] = -686.7561477 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.9196526 a.u.
E[PMP2/6-311++G(2d,p)] = -685.1146306 a.u.
ZPVE = 610.1213 kJ mol^{-1}

Table S3. B3LYP/6-31+G(d,p) optimized structure of **1c**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.138574	1.329338	1.127050
2	1	0	-2.272580	0.647561	1.898308
3	1	0	-2.736492	2.145930	1.268535
4	1	0	-1.138670	1.625334	1.111117
5	6	0	-2.404148	0.599838	-0.167834
6	1	0	-3.392972	0.893431	-0.532558
7	6	0	-1.317104	0.975000	-1.224320
8	6	0	-2.491796	-0.877760	0.230366
9	1	0	-1.379580	0.232611	-2.025394
10	1	0	-1.606670	1.934457	-1.665497
11	6	0	0.068903	1.070467	-0.655571
12	8	0	-2.453898	-1.233748	1.391071
13	6	0	0.719319	2.250257	-0.323114
14	6	0	0.995192	-0.004340	-0.371114
15	1	0	0.399666	3.275822	-0.458268
16	7	0	1.973965	1.966215	0.154410
17	6	0	2.178511	0.596835	0.135386
18	6	0	0.958239	-1.404421	-0.529878

19	1	0	2.662581	2.655258	0.418648
20	6	0	3.302859	-0.150239	0.507855
21	6	0	2.072118	-2.149353	-0.167145
22	1	0	0.087595	-1.896669	-0.952343
23	1	0	4.199146	0.326091	0.892893
24	6	0	3.230077	-1.528684	0.352048
25	1	0	2.060908	-3.227378	-0.291265
26	1	0	4.083627	-2.140826	0.624561
27	8	0	-2.661011	-1.668137	-0.822681
28	1	0	-2.768045	-2.591020	-0.526161

Rotational constants (GHZ): 0.9601849 0.4666515 0.3647595

E[B3LYP/6-31+G(d,p)] = -686.78849884 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.95119281 a.u.
E[PMP2/6-311++G(2d,p)] = -685.15146454 a.u.
ZPVE = 612.1734 kJ mol^{-1}

Table S4. B3LYP/6-31+G(d,p) optimized structure of **1d**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.844951	-1.810462	0.523365
2	1	0	3.499822	-2.058940	-0.229058
3	1	0	2.276872	-2.630154	0.760123
4	1	0	3.398758	-1.567725	1.352604
5	6	0	1.950282	-0.636122	0.088763
6	1	0	1.311038	-1.048006	-0.699510
7	6	0	1.092268	-0.123730	1.261513
8	6	0	2.860335	0.425693	-0.545957
9	1	0	0.841358	-0.981039	1.904194
10	1	0	1.681470	0.574646	1.864631
11	6	0	-0.171497	0.517806	0.773510
12	8	0	2.717648	1.610845	-0.428860
13	6	0	-0.434732	1.865769	0.663669
14	6	0	-1.345999	-0.180200	0.307159
15	1	0	0.194313	2.712022	0.900364
16	7	0	-1.698401	2.045028	0.158481
17	6	0	-2.286945	0.813997	-0.074263
18	6	0	-1.704040	-1.536853	0.186254
19	1	0	-2.131633	2.940793	-0.007698
20	6	0	-3.553470	0.493464	-0.574668
21	6	0	-2.960671	-1.861566	-0.313003
22	1	0	-1.025693	-2.329941	0.495848
23	1	0	-4.263000	1.264861	-0.858185
24	6	0	-3.874388	-0.855019	-0.691937
25	1	0	-3.250908	-2.903281	-0.406111
26	1	0	-4.848939	-1.138973	-1.075542
27	8	0	3.841324	-0.175581	-1.266253
28	1	0	4.392059	0.502238	-1.699926

Rotational constants (GHZ): 1.1638177 0.3524588 0.3017120

E[B3LYP/6-31+G(d,p)] = -686.77328256 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.93533498 a.u.
E[PMP2/6-311++G(2d,p)] = -685.13397855 a.u.
ZPVE = 611.3079 kJ mol^{-1}

Table S5. B3LYP/6-31+G(d,p) optimized structure of **3**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.330718	-0.029130	1.771287
2	1	0	-2.974004	0.530541	2.324046
3	1	0	-2.618628	-1.000444	1.886978
4	6	0	-2.371928	0.341930	0.365150
5	1	0	-2.486449	1.429010	0.285973
6	6	0	-1.053824	-0.088250	-0.328862
7	6	0	-3.542731	-0.299564	-0.394645
8	1	0	-0.995519	-1.181952	-0.327751
9	1	0	-1.035436	0.237909	-1.372325
10	6	0	0.190228	0.423814	0.450953
11	8	0	-4.133081	-1.284717	-0.017269
12	6	0	0.532689	1.854937	0.250158
13	6	0	1.512492	-0.252619	0.180511
14	1	0	-0.117355	2.718167	0.334997
15	7	0	1.800073	1.986419	-0.035840
16	6	0	2.469744	0.734104	-0.096713
17	6	0	1.907629	-1.587001	0.185900
18	1	0	2.258914	2.881295	-0.190232
19	6	0	3.808258	0.474744	-0.370296
20	6	0	3.248875	-1.881467	-0.090182
21	1	0	1.204014	-2.384889	0.400511
22	1	0	4.524396	1.263363	-0.577432
23	6	0	4.184100	-0.870180	-0.363120
24	1	0	3.574703	-2.916492	-0.091721
25	1	0	5.214846	-1.136000	-0.571454
26	8	0	-3.803798	0.352398	-1.545232
27	1	0	-4.537551	-0.099853	-1.999579
28	1	0	-0.115587	0.314202	1.516739

Rotational constants (GHZ): 1.3583769 0.2901573 0.2676393
E[B3LYP/6-31+G(d,p)] = -686.77165773 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.93379586 a.u.
E[PMP2/6-311++G(2d,p)] = -685.12435202 a.u.
ZPVE = 607.5099 kJ mol^{-1}

Table S6. B3LYP/6-31+G(d,p) optimized structure of **4**$^{+}$.
Standard orientation:

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

1	7	0	-2.924129	1.288517	0.163266
2	1	0	-3.662795	1.772636	-0.336718
3	1	0	-3.223281	1.124245	1.122206
4	6	0	-2.550693	0.042343	-0.479788
5	1	0	-3.351902	-0.378468	-1.103874
6	6	0	-1.333140	0.232299	-1.466465
7	6	0	-2.243683	-1.009201	0.586212
8	1	0	-1.151748	-0.710011	-1.986945
9	1	0	-1.653607	0.971917	-2.208187
10	6	0	-0.103486	0.705047	-0.779262
11	8	0	-2.336984	-0.818284	1.777526
12	6	0	0.007902	2.067916	-0.185661
13	6	0	1.058271	0.011464	-0.490685
14	1	0	-0.826882	2.214548	0.525253
15	7	0	1.316861	2.075229	0.437463
16	6	0	1.925208	0.893164	0.272230
17	6	0	1.498086	-1.316864	-0.801336
18	6	0	3.194527	0.462179	0.720437
19	6	0	2.732443	-1.712184	-0.363890
20	1	0	0.860714	-1.984226	-1.370686
21	1	0	3.844691	1.115266	1.292236
22	6	0	3.568550	-0.822229	0.392617
23	1	0	3.099506	-2.708433	-0.584909
24	1	0	4.540270	-1.183099	0.716676
25	8	0	-1.865778	-2.182340	0.040016
26	1	0	-1.742022	-2.826312	0.760134
27	1	0	1.702238	2.863323	0.939717
28	1	0	-0.086112	2.863785	-0.936797

Rotational constants (GHZ): 1.0114915 0.4501159 0.3728297

E[B3LYP/6-31+G(d,p)] = -686.77650807 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.93843559 a.u.
E[PMP2/6-311++G(2d,p)] = -685.12252178 a.u.
ZPVE = 605.4296 kJ mol^{-1}

Table S7. B3LYP/6-31+G(d,p) optimized structure of **5**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.479001	-1.450796	0.780506
2	1	0	-1.699122	-1.686208	1.745835
3	1	0	-1.968145	-2.146925	0.215316
4	6	0	-2.018352	-0.128808	0.453385
5	1	0	-1.926135	0.523368	1.328080
6	6	0	-1.232864	0.519277	-0.722459
7	6	0	-3.504460	-0.194629	0.074527
8	1	0	-1.248155	-0.175372	-1.571155
9	1	0	-1.756144	1.424425	-1.044709
10	6	0	0.188973	0.864777	-0.371169
11	8	0	-4.077208	-1.212876	-0.242689
12	6	0	0.661797	2.156672	-0.066281

13	6	0	1.303175	0.023398	-0.273489
14	1	0	0.110310	3.088147	-0.045618
15	7	0	1.984497	2.129776	0.215205
16	6	0	2.430132	0.819755	0.102751
17	6	0	1.477776	-1.435819	-0.451190
18	1	0	2.547802	2.932946	0.460225
19	6	0	3.683286	0.290075	0.309168
20	6	0	2.857172	-1.931870	-0.222893
21	1	0	0.755361	-1.944658	0.219939
22	1	0	4.518502	0.922550	0.600017
23	6	0	3.889796	-1.115304	0.141618
24	1	0	3.031384	-2.995917	-0.355092
25	1	0	4.882425	-1.519218	0.306814
26	8	0	-4.087649	1.020386	0.108993
27	1	0	-5.019746	0.923392	-0.156823
28	1	0	1.133469	-1.764611	-1.447048

Rotational constants (GHZ): 1.3257506 0.3282643 0.2738751

E[B3LYP/6-31+G(d,p)] = -686.76394344 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.92582599 a.u.
E[PMP2/6-311++G(2d,p)] = -685.11169166 a.u.
ZPVE = 604.7671 kJ mol^{-1}

Table S8. B3LYP/6-31+G(d,p) optimized structure of **6**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.638671	-0.834789	0.187676
2	1	0	1.361339	-1.785158	-0.256964
3	6	0	1.283797	-0.582445	1.599385
4	6	0	2.881051	-0.188543	-0.362697
5	1	0	0.781495	-1.361252	2.163602
6	1	0	1.920426	0.088465	2.167110
7	6	0	0.411898	0.078268	0.501693
8	8	0	3.248210	0.932878	-0.075912
9	6	0	0.451518	1.520480	0.316925
10	6	0	-0.991046	-0.305769	0.199263
11	1	0	1.303319	2.178824	0.429864
12	7	0	-0.743362	1.941416	-0.025929
13	6	0	-1.677655	0.876971	-0.120260
14	6	0	-1.679307	-1.516262	0.185539
15	1	0	-0.970797	2.916538	-0.199357
16	6	0	-3.026260	0.921766	-0.455537
17	6	0	-3.037789	-1.498168	-0.150737
18	1	0	-1.188210	-2.454345	0.425428
19	1	0	-3.533076	1.850521	-0.696689
20	6	0	-3.700843	-0.301099	-0.465549
21	1	0	-3.591951	-2.430750	-0.168540
22	1	0	-4.754705	-0.324865	-0.721070
23	8	0	3.527506	-1.020379	-1.184334
24	1	0	4.345756	-0.590345	-1.494121

Rotational constants (GHZ):	1.6115271	0.4384527	0.3863094

E[B3LYP/6-31+G(d,p)] = -630.18469259 a.u.
E[B3LYP/6-311++G(2d,p)] = -630.33095966 a.u.
E[PMP2/6-311++G(2d,p)] = -628.67576485 a.u.
ZPVE = 502.7873 kJ mol^{-1}

Table S9. B3LYP/6-31+G(d,p) optimized structure of **7**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.490868	2.375055	1.277337
2	1	0	4.027772	2.225260	2.129864
3	1	0	3.281900	3.371071	1.247821
4	1	0	4.122955	2.184688	0.501831
5	6	0	1.196393	-1.088575	0.392909
6	1	0	0.750419	-2.038182	0.672017
7	6	0	1.148977	0.021669	1.366744
8	6	0	2.353073	-1.183681	-0.563932
9	1	0	0.681149	-0.165019	2.328460
10	1	0	1.924769	0.792271	1.334245
11	6	0	0.142837	0.038396	0.178267
12	8	0	2.826770	-0.249124	-1.177777
13	6	0	0.290489	1.055404	-0.845170
14	6	0	-1.321260	-0.172304	0.299727
15	1	0	1.210576	1.476223	-1.227416
16	7	0	-0.900346	1.418563	-1.266400
17	6	0	-1.935751	0.704137	-0.609675
18	6	0	-2.116946	-1.002368	1.086530
19	1	0	-1.058440	2.130630	-1.972958
20	6	0	-3.312444	0.800647	-0.780023
21	6	0	-3.505296	-0.925360	0.932406
22	1	0	-1.683658	-1.693615	1.802775
23	1	0	-3.761528	1.488061	-1.489586
24	6	0	-4.094260	-0.039517	0.015526
25	1	0	-4.142341	-1.564254	1.535054
26	1	0	-5.174467	-0.006047	-0.077178
27	8	0	2.803556	-2.442706	-0.630864
28	1	0	3.569761	-2.472460	-1.232218

Rotational constants (GHZ):	0.9962466	0.3510012	0.3172375

E[B3LYP/6-31+G(d,p)] = -686.76454944 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.92627499 a.u.
E[PMP2/6-311++G(2d,p)] = -685.117035 a.u.
ZPVE = 598.6111 kJ mol^{-1}

Table S10. B3LYP/6-31+G(d,p) optimized structure of **8**$^{+}$.
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.989245	-0.882418	0.125277
2	1	0	1.914643	-1.830940	-0.396257
3	6	0	1.617704	-0.829594	1.559469
4	6	0	3.054594	0.052325	-0.370630
5	1	0	1.316146	-1.747015	2.053698
6	1	0	2.117347	-0.092056	2.179234
7	6	0	0.610022	-0.283487	0.531114
8	8	0	3.205895	1.191061	0.024900
9	6	0	0.325410	1.148325	0.457104
10	6	0	-0.685465	-0.931159	0.198119
11	1	0	1.021954	1.959759	0.624649
12	7	0	-0.929377	1.341160	0.148340
13	6	0	-1.606068	0.105803	-0.027155
14	6	0	-1.102078	-2.255054	0.090547
15	1	0	-1.376149	2.309541	0.045569
16	6	0	-2.938458	-0.117182	-0.358821
17	6	0	-2.439020	-2.501051	-0.244339
18	1	0	-0.419869	-3.083125	0.258194
19	1	0	-3.634144	0.697965	-0.526723
20	6	0	-3.342730	-1.450491	-0.465186
21	1	0	-2.784093	-3.525796	-0.334359
22	1	0	-4.372153	-1.676406	-0.722171
23	8	0	3.824553	-0.541641	-1.290649
24	1	0	4.524594	0.079084	-1.563166
25	1	0	-2.458446	4.031119	-1.060809
26	7	0	-2.048889	3.892126	-0.137607
27	1	0	-1.357147	4.631696	-0.019204
28	1	0	-2.787356	4.081711	0.539216

Rotational constants (GHZ): 0.7771506 0.4210481 0.3003486
E[B3LYP/6-31+G(d,p)] = -686.7824895 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.94333714 a.u.
E[PMP2/6-311++G(2d,p)] = -685.1354365 a.u.
ZPVE = 599.7901 kJ mol^{-1}

Table S11. B3LYP/6-31+G(d,p) optimized structure of **9**$^{+}$.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.038983	-0.850109	0.501258
2	1	0	0.814553	-1.787557	0.002231
3	6	0	0.502980	-0.628242	1.854784
4	6	0	2.354144	-0.199645	0.122415
5	1	0	-0.078406	-1.409742	2.332913
6	1	0	1.055791	0.033094	2.514123
7	6	0	-0.223278	0.062516	0.667461
8	8	0	2.642024	0.935664	0.485249
9	6	0	-0.151848	1.501471	0.511251
10	6	0	-1.574598	-0.308845	0.180528

11	1	0	0.686788	2.145260	0.742142
12	7	0	-1.288248	1.938068	0.014005
13	6	0	-2.206322	0.881403	-0.216238
14	6	0	-2.262515	-1.514884	0.062046
15	1	0	-1.483417	2.915647	-0.179096
16	6	0	-3.497579	0.936914	-0.729473
17	6	0	-3.562841	-1.485361	-0.452891
18	1	0	-1.812086	-2.457780	0.356674
19	1	0	-3.962652	1.871032	-1.027523
20	6	0	-4.171275	-0.280949	-0.842407
21	1	0	-4.114774	-2.414036	-0.553684
22	1	0	-5.181590	-0.295414	-1.236888
23	8	0	3.102926	-1.004847	-0.587013
24	1	0	4.049771	-0.585079	-0.801401
25	1	0	5.634158	0.091689	-2.116953
26	7	0	5.460758	-0.016494	-1.119217
27	1	0	6.210092	-0.595010	-0.743245
28	1	0	5.539506	0.904728	-0.691101

Rotational constants (GHZ): 1.4236030 0.2883121 0.2704724

E[B3LYP/6-31+G(d,p)] = -686.78292366 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.94334001 a.u.
E[PMP2/6-311++G(2d,p)] = -685.1332923 a.u.
ZPVE = 598.8881 kJ mol^{-1}

Table S12. B3LYP/6-31+G(d,p) optimized structure of **TS1**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.802377	-0.935336	1.508097
2	1	0	2.213845	-1.696302	2.042240
3	1	0	1.868865	-0.063481	2.039946
4	6	0	2.368372	-0.770692	0.162069
5	1	0	3.232716	-1.421556	0.010477
6	6	0	1.241357	-1.156674	-0.883704
7	6	0	2.837266	0.670745	-0.007644
8	1	0	1.267450	-0.493585	-1.751101
9	1	0	1.440642	-2.166908	-1.250401
10	6	0	-0.118845	-1.124731	-0.180192
11	8	0	2.626126	1.546441	0.804732
12	6	0	-0.997696	-2.257358	-0.209835
13	6	0	-1.040837	0.042031	-0.139259
14	1	0	-0.739439	-3.306910	-0.282435
15	7	0	-2.261474	-1.867111	-0.085811
16	6	0	-2.352657	-0.463388	-0.038079
17	6	0	-0.850411	1.428088	-0.124563
18	1	0	-3.052714	-2.496875	-0.015623
19	6	0	-3.485210	0.341174	0.076482
20	6	0	-1.973085	2.250958	-0.024101
21	1	0	0.140321	1.865718	-0.183175
22	1	0	-4.483243	-0.077330	0.158476

23	6	0	-3.271216	1.717708	0.078113
24	1	0	-1.842847	3.328234	-0.021125
25	1	0	-4.119556	2.388895	0.159847
26	8	0	3.489610	0.839773	-1.163338
27	1	0	3.778651	1.767438	-1.235482
28	1	0	0.440878	-1.167076	0.985488

Rotational constants (GHZ): 1.0463036 0.4194797 0.3355669
E[B3LYP/6-31+G(d,p)] = -686.76628543 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.92777803 a.u.
E[PMP2/6-311++G(2d,p)] = -685.1223228 a.u.
ZPVE = 598.7151 kJ mol^{-1}

Table S13. B3LYP/6-31+G(d,p) optimized structure of **TS2**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.336270	1.400528	0.649536
2	1	0	-2.386344	1.062193	1.615379
3	1	0	-3.046510	2.113551	0.496685
4	1	0	-1.008210	1.885352	0.413587
5	6	0	-2.440751	0.267926	-0.284395
6	1	0	-3.440552	0.212585	-0.726901
7	6	0	-1.412438	0.418393	-1.480589
8	6	0	-2.222039	-1.015530	0.521916
9	1	0	-1.386491	-0.523463	-2.030323
10	1	0	-1.803800	1.188699	-2.152675
11	6	0	-0.082730	0.807564	-0.938932
12	8	0	-2.050629	-1.023493	1.721186
13	6	0	0.090942	2.093511	-0.320916
14	6	0	1.010998	0.001329	-0.564095
15	1	0	-0.196230	3.030116	-0.799157
16	7	0	1.345188	2.062067	0.324657
17	6	0	1.897966	0.825374	0.207839
18	6	0	1.352027	-1.357187	-0.809068
19	1	0	1.782518	2.854649	0.772602
20	6	0	3.105974	0.322378	0.730772
21	6	0	2.541028	-1.834703	-0.306568
22	1	0	0.698718	-1.993458	-1.397361
23	1	0	3.773948	0.945984	1.315599
24	6	0	3.406997	-0.997786	0.457421
25	1	0	2.835610	-2.862046	-0.492327
26	1	0	4.335503	-1.415720	0.833785
27	8	0	-2.266706	-2.105076	-0.253265
28	1	0	-2.169741	-2.895671	0.308063

Rotational constants (GHZ): 0.9635161 0.4867617 0.3930876
E[B3LYP/6-31+G(d,p)] = -686.76588398 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.92709514v
E[PMP2/6-311++G(2d,p)] = -685.12023453 a.u.
ZPVE = 597.8095 kJ mol^{-1}

Table S14. B3LYP/6-31+G(d,p) optimized structure of **TS3**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.237407	-1.344656	-0.663791
2	1	0	1.266739	-1.580144	-1.655487
3	1	0	1.806718	-2.055309	-0.191867
4	6	0	1.878827	-0.018272	-0.430939
5	1	0	1.791257	0.573913	-1.346627
6	6	0	1.216651	0.784846	0.726402
7	6	0	3.367380	-0.236424	-0.132916
8	1	0	1.317028	0.219468	1.662085
9	1	0	1.784539	1.709883	0.856779
10	6	0	-0.230510	1.084291	0.443825
11	8	0	3.839951	-1.318583	0.139765
12	6	0	-0.819206	2.284462	0.057742
13	6	0	-1.259606	0.117681	0.400433
14	1	0	-0.380574	3.270472	-0.019233
15	7	0	-2.139051	2.085667	-0.248197
16	6	0	-2.438485	0.744618	-0.087269
17	6	0	-1.218231	-1.317160	0.586833
18	1	0	-2.773538	2.801665	-0.572293
19	6	0	-3.578232	0.011797	-0.390637
20	6	0	-2.431711	-2.032337	0.280877
21	1	0	-0.204537	-1.518684	-0.154792
22	1	0	-4.474241	0.494381	-0.771802
23	6	0	-3.554555	-1.391076	-0.218160
24	1	0	-2.467635	-3.101524	0.468119
25	1	0	-4.444658	-1.962680	-0.456886
26	8	0	4.059351	0.909785	-0.184406
27	1	0	4.991675	0.727166	0.032661
28	1	0	-0.689614	-1.689864	1.473238

Rotational constants (GHZ): 1.2601988 0.3590804 0.2924794
E[B3LYP/6-31+G(d,p)] = -686.75680038 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.91788724 a.u.
E[PMP2/6-311++G(2d,p)] = -685.10703855 a.u.
ZPVE = 596.6705 kJ mol^{-1}

Table S15. B3LYP/6-31+G(d,p) optimized structure of **TS4**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.309410	-1.905300	0.351784
2	1	0	2.939895	-2.297008	-0.358495
3	1	0	1.473092	-2.494974	0.424250
4	1	0	2.800919	-1.943986	1.251395
5	6	0	1.910438	-0.470427	-0.005471

6	1	0	1.284500	-0.570600	-0.898340
7	6	0	1.092781	0.194223	1.139460
8	6	0	3.160179	0.312772	-0.418568
9	1	0	0.939275	-0.548301	1.937591
10	1	0	1.691178	1.000700	1.570360
11	6	0	-0.226746	0.714670	0.661813
12	8	0	3.220855	1.511113	-0.413884
13	6	0	-0.568481	2.029967	0.437062
14	6	0	-1.369377	-0.084873	0.295303
15	1	0	0.014908	2.928365	0.583866
16	7	0	-1.853165	2.093307	-0.046558
17	6	0	-2.374721	0.816155	-0.150199
18	6	0	-1.653056	-1.464389	0.308913
19	1	0	-2.341638	2.945110	-0.278174
20	6	0	-3.630186	0.378971	-0.586149
21	6	0	-2.897633	-1.906125	-0.126692
22	1	0	-0.931764	-2.187479	0.690613
23	1	0	-4.389923	1.079196	-0.919683
24	6	0	-3.874284	-0.990640	-0.573339
25	1	0	-3.130779	-2.966044	-0.112834
26	1	0	-4.838289	-1.362680	-0.904529
27	8	0	4.150134	-0.521410	-0.821934
28	1	0	4.913516	0.002195	-1.128847

Rotational constants (GHZ): 1.2068722 0.3413203 0.2853026
E[B3LYP/6-31+G(d,p)] = -686.7723503 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.934386 a.u.
E[PMP2/6-311++G(2d,p)] = -685.1321851 a.u.
ZPVE = 611.3645 kJ mol^{-1}

Table S16. B3LYP/6-31+G(d,p) optimized structure of **TS5**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.441177	1.967005	0.034718
2	1	0	3.822535	2.045426	0.975804
3	1	0	3.158820	2.894672	-0.275104
4	1	0	4.177937	1.634871	-0.585395
5	6	0	1.644311	0.581050	-0.002384
6	1	0	1.200902	1.194221	0.771270
7	6	0	1.102359	0.608093	-1.362571
8	6	0	2.527030	-0.555040	0.423257
9	1	0	0.784863	1.587095	-1.720186
10	1	0	1.708377	0.079842	-2.097420
11	6	0	-0.040594	-0.200169	-0.802203
12	8	0	2.989170	-1.376141	-0.340194
13	6	0	-0.104585	-1.606051	-0.714620
14	6	0	-1.322538	0.299524	-0.325521
15	1	0	0.649316	-2.337556	-0.971026
16	7	0	-1.313053	-1.964545	-0.247284
17	6	0	-2.099495	-0.833368	0.007348

18	6	0	-1.882746	1.576708	-0.185969
19	1	0	-1.607084	-2.920774	-0.094972
20	6	0	-3.406998	-0.744246	0.482100
21	6	0	-3.188796	1.680577	0.290320
22	1	0	-1.323296	2.471210	-0.444171
23	1	0	-3.990010	-1.626632	0.725983
24	6	0	-3.939528	0.536771	0.621665
25	1	0	-3.639399	2.661032	0.404020
26	1	0	-4.954605	0.653234	0.986401
27	8	0	2.764782	-0.518503	1.745970
28	1	0	3.352637	-1.259810	1.978025

Rotational constants (GHZ): 1.1574615 0.3670634 0.3195696

E[B3LYP/6-31+G(d,p)] = -686.74992899 a.u.
E[B3LYP/6-311++G(2d,p)] = -686.91186564 a.u.
E[PMP2/6-311++G(2d,p)] = -685.10267626 a.u.
ZPVE = 599.1888 kJ mol^{-1}

Table S17. B3LYP/6-31++G(d,p) optimized structure of **3**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.626475	0.413299	-1.721688
2	1	0	3.437551	0.994378	-1.916217
3	1	0	2.854520	-0.518252	-2.063749
4	6	0	2.358399	0.364562	-0.290168
5	1	0	2.313555	1.390260	0.094105
6	6	0	0.996095	-0.307485	-0.003594
7	6	0	3.446208	-0.367901	0.498550
8	1	0	1.026007	-1.337413	-0.384641
9	1	0	0.842153	-0.361001	1.078593
10	6	0	-0.197440	0.437434	-0.651869
11	8	0	4.239419	-1.158502	0.029416
12	6	0	-0.411261	1.846390	-0.136674
13	6	0	-1.541292	-0.209669	-0.343434
14	1	0	0.127293	2.721594	-0.479879
15	7	0	-1.754489	1.986141	0.222611
16	6	0	-2.413243	0.761994	0.187152
17	6	0	-1.987504	-1.515187	-0.504174
18	1	0	-2.120064	2.796210	0.699513
19	6	0	-3.718069	0.448936	0.574297
20	6	0	-3.299339	-1.848660	-0.127903
21	1	0	-1.331521	-2.277401	-0.917119
22	1	0	-4.381780	1.203441	0.987157
23	6	0	-4.147972	-0.872703	0.407306
24	1	0	-3.655088	-2.866876	-0.250696
25	1	0	-5.159321	-1.141380	0.698960
26	8	0	3.426671	-0.053079	1.817602
27	1	0	4.118209	-0.581168	2.252401
28	1	0	-0.011623	0.447926	-1.737967

Rotational constants (GHZ): 1.0539375 0.4195994 0.3536045
E[B3LYP/6-31++G(d,p)] = -686.9666478 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.1290992 a.u.
E[PMP2/6-311++G(2d,p)] = -685.3105582 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.3106225 a.u.
ZPVE = 598.2406 kJ mol^{-1}

Table S18. B3LYP/6-31++G(d,p) optimized structure of **4**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.120936	1.225592	-0.127206
2	1	0	-3.748402	1.636426	-0.810118
3	1	0	-3.619527	1.104418	0.750284
4	6	0	-2.584172	-0.047796	-0.599509
5	1	0	-3.289412	-0.593508	-1.250672
6	6	0	-1.279705	0.159962	-1.427207
7	6	0	-2.354786	-0.965608	0.592998
8	1	0	-1.027956	-0.785002	-1.918155
9	1	0	-1.542769	0.871717	-2.225294
10	6	0	-0.102807	0.659833	-0.654841
11	8	0	-2.665964	-0.714243	1.738996
12	6	0	-0.021751	2.031799	-0.033018
13	6	0	1.120766	-0.002063	-0.434758
14	1	0	-0.732158	2.151838	0.799373
15	7	0	1.373650	2.116257	0.418430
16	6	0	1.998137	0.891596	0.271380
17	6	0	1.590349	-1.298214	-0.764004
18	6	0	3.274605	0.501418	0.664562
19	6	0	2.872228	-1.679443	-0.374057
20	1	0	0.949432	-1.991892	-1.299495
21	1	0	3.928865	1.184900	1.198544
22	6	0	3.703701	-0.795769	0.338367
23	1	0	3.235031	-2.673634	-0.618448
24	1	0	4.697321	-1.117340	0.636243
25	8	0	-1.786921	-2.136891	0.229376
26	1	0	-1.655497	-2.658952	1.038985
27	1	0	1.615785	2.721766	1.188807
28	1	0	-0.256020	2.831097	-0.755071

Rotational constants (GHZ): 1.0539375 0.4195994 0.3536045
E[B3LYP/6-31++G(d,p)] = -686.97864536 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.1415638 a.u.
E[PMP2/6-311++G(2d,p)] = -685.3201114 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.3227536 a.u.
ZPVE = 598.0007 kJ mol^{-1}

Table S19. B3LYP/6-31++G(d,p) optimized structure of **5**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.600171	-1.469426	0.911914
2	1	0	-1.979498	-1.688269	1.829316
3	1	0	-1.943087	-2.190225	0.279104
4	6	0	-2.063816	-0.164159	0.461428
5	1	0	-1.953102	0.552075	1.281753
6	6	0	-1.211256	0.350560	-0.737174
7	6	0	-3.537199	-0.170290	0.047212
8	1	0	-1.178782	-0.447826	-1.489706
9	1	0	-1.735825	1.195226	-1.197152
10	6	0	0.180884	0.781359	-0.364572
11	8	0	-4.164930	-1.150504	-0.297600
12	6	0	0.551813	2.091430	-0.079352
13	6	0	1.355056	-0.012320	-0.245196
14	1	0	-0.039640	2.996157	-0.074301
15	7	0	1.896552	2.117520	0.212692
16	6	0	2.413142	0.839458	0.112246
17	6	0	1.585126	-1.482945	-0.440531
18	1	0	2.427448	2.942647	0.441452
19	6	0	3.744737	0.407638	0.310235
20	6	0	3.026465	-1.871848	-0.226411
21	1	0	0.930576	-2.053734	0.237943
22	1	0	4.535144	1.097927	0.586344
23	6	0	4.006009	-0.975795	0.125571
24	1	0	3.280921	-2.920615	-0.354927
25	1	0	5.022419	-1.334069	0.269189
26	8	0	-4.086089	1.070736	0.075716
27	1	0	-5.004446	0.989250	-0.234866
28	1	0	1.265588	-1.795580	-1.452056

Rotational constants (GHZ): 1.3522487 0.3169185 0.2680471

E[B3LYP/6-31++G(d,p)] = -686.97180533 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.13455569 a.u.
E[PMP2/6-311++G(2d,p)] = -685.3163031 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.3195421 a.u.
ZPVE = 596.7981 kJ mol^{-1}

Table S20. B3LYP/6-31++G(d,p) optimized structure of **11**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.043065	1.853456	-0.396162
2	1	0	4.215632	-0.013875	-0.443882
3	1	0	3.464370	2.369782	0.372486
4	1	0	2.630866	2.527633	-1.034865
5	6	0	2.029166	0.902997	0.110932
6	1	0	1.337268	1.350617	0.837482
7	6	0	1.203623	0.384028	-1.107024
8	6	0	2.826666	-0.164712	0.824707

9	1	0	0.947237	1.259063	-1.722547
10	1	0	1.854698	-0.246478	-1.722150
11	6	0	-0.058408	-0.349135	-0.764345
12	8	0	3.845441	-0.741382	0.091035
13	6	0	-0.273342	-1.702980	-0.843142
14	6	0	-1.297279	0.230209	-0.299531
15	1	0	0.408838	-2.487867	-1.138244
16	7	0	-1.565851	-2.003827	-0.451786
17	6	0	-2.220484	-0.836741	-0.111644
18	6	0	-1.723180	1.545419	-0.034621
19	1	0	-1.961642	-2.929152	-0.416444
20	6	0	-3.531798	-0.624869	0.329213
21	6	0	-3.025472	1.762766	0.403886
22	1	0	-1.045915	2.384459	-0.170513
23	1	0	-4.223412	-1.451655	0.466639
24	6	0	-3.921137	0.686927	0.585771
25	1	0	-3.361757	2.774468	0.611185
26	1	0	-4.931620	0.885639	0.930498
27	8	0	2.099737	-1.086706	1.524768
28	1	0	2.713377	-1.748785	1.874347

Rotational constants (GHZ): 1.2050723 0.3590670 0.3122129
E[B3LYP/6-31++G(d,p)] = -686.95335571 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.11458155 a.u.
E[PMP2/6-311++G(2d,p)] = -685.3011147 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2961074
ZPVE = 600.6753 kJ mol^{-1}

Table S21. B3LYP/6-31++G(d,p) optimized structure of **1**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.183721	1.295534	1.172994
2	1	0	-2.710416	0.686604	1.829544
3	1	0	-2.583324	2.261622	1.187433
4	1	0	-1.188885	1.311525	1.439245
5	6	0	-2.365399	0.636251	-0.187598
6	1	0	-3.320113	1.113042	-0.544263
7	6	0	-1.241773	1.013682	-1.178354
8	6	0	-2.583302	-0.799351	0.141131
9	1	0	-1.299844	0.295200	-2.002686
10	1	0	-1.492586	1.995853	-1.597280
11	6	0	0.155899	1.073490	-0.621323
12	8	0	-3.197701	-1.145546	1.177887
13	6	0	0.842244	2.234948	-0.335838
14	6	0	1.061859	-0.014773	-0.322127
15	1	0	0.526747	3.263214	-0.451451
16	7	0	2.108655	1.936651	0.126744
17	6	0	2.275058	0.564420	0.142275
18	6	0	0.971560	-1.417339	-0.417741
19	1	0	2.807379	2.614657	0.386013

20	6	0	3.381879	-0.207278	0.517181
21	6	0	2.070031	-2.186792	-0.052066
22	1	0	0.057569	-1.882626	-0.770731
23	1	0	4.300016	0.252813	0.871668
24	6	0	3.261839	-1.589123	0.413361
25	1	0	2.012982	-3.268979	-0.121864
26	1	0	4.100734	-2.219156	0.693781
27	8	0	-2.411554	-1.653986	-0.924082
28	1	0	-2.790126	-2.501630	-0.641418

Rotational constants (GHZ): 0.9812413 0.4379135 0.3458361

E[B3LYP/6-31++G(d,p)] = -686.92572555 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.08704223 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2665938 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2653942 a.u.
ZPVE = 597.1285 kJ mol^{-1}

Table S22. B3LYP/6-31++G(d,p) optimized structure of **12**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.153387	1.806825	-0.591196
2	1	0	3.761702	-1.660129	0.948253
3	1	0	3.822494	1.232729	-1.101189
4	1	0	3.676464	2.250835	0.160418
5	6	0	2.105363	0.949301	-0.022485
6	1	0	1.445323	1.587429	0.576350
7	6	0	1.271750	0.361160	-1.201683
8	6	0	2.640166	-0.109859	0.915116
9	1	0	1.026940	1.206881	-1.855009
10	1	0	1.918016	-0.310482	-1.778878
11	6	0	0.012411	-0.360905	-0.809556
12	8	0	3.593143	-0.930611	0.334809
13	6	0	-0.227583	-1.715537	-0.890859
14	6	0	-1.217434	0.235025	-0.330755
15	1	0	0.429177	-2.507845	-1.223137
16	7	0	-1.521154	-1.995702	-0.486388
17	6	0	-2.153883	-0.817776	-0.137660
18	6	0	-1.618916	1.558050	-0.064722
19	1	0	-1.933903	-2.914147	-0.455159
20	6	0	-3.457378	-0.587557	0.319412
21	6	0	-2.913292	1.793068	0.385013
22	1	0	-0.929921	2.384761	-0.212166
23	1	0	-4.159957	-1.403553	0.463827
24	6	0	-3.822408	0.729862	0.578174
25	1	0	-3.233977	2.809536	0.592446
26	1	0	-4.826099	0.944467	0.932797
27	8	0	1.775005	-0.767547	1.757981
28	1	0	0.920156	-0.922069	1.312246

Rotational constants (GHZ): 1.1653421 0.3759051 0.3314897

E[B3LYP/6-31++G(d,p)] = -686.9455574 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.1073547 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2956858 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2945054 a.u.
ZPVE = 597.7666 kJ mol^{-1}

Table S23. B3LYP/6-31++G(d,p) optimized structure of **13**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.833179	0.453669	-0.728897
2	1	0	2.015368	-2.602353	0.747077
3	1	0	3.851775	-0.366794	-1.332118
4	1	0	4.595667	0.334846	-0.065386
5	6	0	2.554060	0.502683	-0.006653
6	1	0	2.591472	1.358843	0.677091
7	6	0	1.429336	0.779774	-1.050797
8	6	0	2.305813	-0.714548	0.854177
9	1	0	1.758903	1.651489	-1.625891
10	1	0	1.395769	-0.063161	-1.750882
11	6	0	0.054214	1.019577	-0.485682
12	8	0	2.320220	-1.904931	0.148588
13	6	0	-0.418267	2.198417	0.047548
14	6	0	-1.048439	0.082834	-0.421402
15	1	0	0.085146	3.147853	0.168765
16	7	0	-1.735532	2.049390	0.443254
17	6	0	-2.152654	0.763354	0.165867
18	6	0	-1.213712	-1.258900	-0.820401
19	1	0	-2.301161	2.771233	0.860464
20	6	0	-3.393571	0.145907	0.368513
21	6	0	-2.444668	-1.873900	-0.625212
22	1	0	-0.388031	-1.804105	-1.268014
23	1	0	-4.225191	0.680457	0.819104
24	6	0	-3.523924	-1.178780	-0.034914
25	1	0	-2.583283	-2.906914	-0.930113
26	1	0	-4.472950	-1.687504	0.105524
27	8	0	1.376088	-0.663228	1.864493
28	1	0	0.533387	-0.288545	1.542973

Rotational constants (GHZ): 1.0842683 0.4197356 0.3546654
E[B3LYP/6-31++G(d,p)] = -686.9444005 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.1060671 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2951427 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2939392 a.u.
ZPVE = 597.1915 kJ mol^{-1}

Table S24. B3LYP/6-31++G(d,p) optimized structure of **16**
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.560006	-1.423191	0.000004
2	1	0	2.220931	-2.452283	0.000006
3	1	0	3.629735	-1.245895	0.000003
4	6	0	1.650954	-0.360420	0.000001
5	6	0	1.947062	1.015732	-0.000005
6	6	0	0.187765	-0.435428	-0.000001
7	1	0	2.909473	1.506654	-0.000008
8	7	0	0.777341	1.748225	0.000001
9	6	0	-0.312290	0.890586	0.000001
10	6	0	-0.718784	-1.503416	-0.000003
11	1	0	0.725294	2.754184	0.000003
12	6	0	-1.681295	1.174328	0.000002
13	6	0	-2.086639	-1.233318	0.000000
14	1	0	-0.362378	-2.529589	-0.000004
15	1	0	-2.049027	2.196610	0.000004
16	6	0	-2.561146	0.093181	0.000000
17	1	0	-2.797892	-2.053737	0.000001
18	1	0	-3.631320	0.278157	0.000001

Rotational constants (GHZ): 2.6879684 1.2929875 0.8730339
E[B3LYP/6-31++G(d,p)] = -402.51687712 a.u.
E[B3LYP/6-311++G(2d,p)] = -402.60224833 a.u.
E[PMP2/6-311++G(2d,p)] = -401.4546143 a.u.
E[ROMP2/6-311++G(2d,p)] = -401.4582138 a.u.
ZPVE = 377.4322 kJ mol^{-1}

Table S25. B3LYP/6-31+G(d,p) optimized structure of **17**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.873594	0.055425	0.000178
2	1	0	2.452544	-0.100885	-0.821090
3	1	0	2.452709	-0.101833	0.821153
4	6	0	0.679691	-0.750771	-0.000160
5	1	0	0.698998	-1.835533	-0.000327
6	6	0	-0.482141	-0.073268	-0.000026
7	8	0	-0.541804	1.280398	-0.000042
8	8	0	-1.699657	-0.656758	-0.000033
9	1	0	-2.370030	0.041394	0.000991
10	1	0	0.397002	1.563995	-0.000255

Rotational constants (GHZ): 10.7042937 3.9471717 2.9292172
E[B3LYP/6-31++G(d,p)] = -284.4209663 a.u.
E[B3LYP/6-311++G(2d,p)] = -284.5000951 a.u.
E[PMP2/6-311++G(2d,p)] = -283.5054241 a.u.
ZPVE = 207.6566

Table S26. B3LYP/6-31++G(d,p) optimized structure of **15**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.509309	-1.028776	0.289205
2	1	0	-2.093857	-1.060295	-0.679163
3	1	0	1.447034	-1.439694	-0.638371
4	1	0	1.183673	-1.725007	0.953252
5	6	0	0.715960	0.190410	0.368064
6	1	0	0.770630	0.554289	1.409440
7	6	0	1.266337	1.245622	-0.541229
8	6	0	-0.796931	0.063822	0.099461
9	1	0	2.317979	1.204822	-0.800607
10	1	0	0.673864	2.117675	-0.791106
11	8	0	-1.132862	-1.087945	-0.530909
12	8	0	-1.614223	0.906760	0.401451

Rotational constants (GHZ): 5.2109258 3.1591652 2.2981891

E[B3LYP/6-31++G(d,p)] = -323.1011077 a.u.

E[B3LYP/6-311++G(2d,p)] = -323.1875075 a.u.

E[PMP2/6-311++G(2d,p)] = -322.3841810 a.u.

ZPVE = 244.2838 kJ mol^{-1}

Table S27. B3LYP/6-31++G(d,p) optimized structure of **14**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.930928	-0.532047	0.000000
2	6	0	-2.254735	0.800996	0.000000
3	6	0	-0.494974	-0.618519	0.000000
4	1	0	-3.222906	1.281333	0.000000
5	7	0	-1.096108	1.558224	0.000000
6	6	0	0.000000	0.716450	0.000000
7	6	0	0.426702	-1.682801	0.000000
8	1	0	-1.059987	2.564788	0.000000
9	6	0	1.369641	1.008096	0.000000
10	6	0	1.787611	-1.398816	0.000000
11	1	0	0.077376	-2.711728	0.000000
12	1	0	1.730973	2.032910	0.000000
13	6	0	2.254844	-0.065576	0.000000
14	1	0	2.507073	-2.212397	0.000000
15	1	0	3.324072	0.124713	0.000000
16	1	0	-2.632812	-1.353888	0.000000

Rotational constants (GHZ): 3.8719574 1.6285050 1.1463585

E[B3LYP/6-31++G(d,p)] = -363.8450950 a.u.

E[B3LYP/6-311++G(2d,p)] = -363.9227811 a.u.

E[PMP2/6-311++G(2d,p)] = -362.8984954 a.u.

E[ROMP2/6-311++G(2d,p)] = -322.382509 a.u.

ZPVE = 340.4392 kJ mol^{-1}

Table S28. B3LYP/6-31++G(d,p) optimized structure of **TS6**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.379573	-1.269852	-1.180400
2	1	0	-3.610577	1.318650	1.609654
3	1	0	-3.971177	-0.462241	-1.364066
4	1	0	-3.962153	-1.951906	-0.700795
5	6	0	-2.259319	-0.882572	-0.331987
6	1	0	-1.723017	-1.791456	-0.039292
7	6	0	-1.274759	0.012966	-1.159834
8	6	0	-2.573866	-0.128835	0.938519
9	1	0	-0.920692	-0.597997	-1.994481
10	1	0	-1.859412	0.837292	-1.585269
11	6	0	-0.080237	0.595225	-0.392419
12	8	0	-3.669790	0.709290	0.857443
13	6	0	0.368120	1.942605	-0.612467
14	6	0	1.183285	-0.158937	-0.170306
15	1	0	-0.217276	2.823858	-0.831698
16	7	0	1.714722	2.034786	-0.352805
17	6	0	2.243480	0.775563	-0.099665
18	6	0	1.463224	-1.514876	0.016889
19	1	0	2.242296	2.893768	-0.342111
20	6	0	3.562579	0.396632	0.165228
21	6	0	2.779713	-1.911084	0.270824
22	1	0	0.671943	-2.256770	-0.032243
23	1	0	4.363253	1.128655	0.221064
24	6	0	3.814621	-0.963119	0.349542
25	1	0	3.006372	-2.963267	0.412768
26	1	0	4.828879	-1.293076	0.553791
27	8	0	-1.567548	0.216609	1.661903
28	1	0	-0.656815	0.571349	0.824409

Rotational constants (GHZ): 1.2257117 0.3666142 0.3293268

E[B3LYP/6-31++G(d,p)] = -686.9093901 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.0706195 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2505016 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2405042 a.u.
ZPVE = 584.1458 kJ mol^{-1}

Table S29. B3LYP/6-31++G(d,p) optimized structure of **TS7**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.105385	2.003757	-0.066047
2	1	0	-3.951991	-1.680555	-0.204542
3	1	0	-3.773023	1.691205	0.635680
4	1	0	-3.635889	2.154743	-0.921214
5	6	0	-2.085752	0.978006	-0.282042

6	1	0	-1.451051	1.299310	-1.116087
7	6	0	-1.180804	0.870708	0.975677
8	6	0	-2.628082	-0.394536	-0.667239
9	1	0	-0.842838	1.882355	1.226199
10	1	0	-1.787628	0.515487	1.819707
11	6	0	0.002045	-0.040350	0.756653
12	8	0	-3.764484	-0.757045	0.022938
13	6	0	-0.066817	-1.468993	0.710837
14	6	0	1.302350	0.335357	0.332123
15	1	0	-0.656390	-2.059000	1.414138
16	7	0	1.245112	-1.928146	0.431657
17	6	0	2.057260	-0.864732	0.127043
18	6	0	1.927496	1.583719	0.096489
19	1	0	1.478288	-2.891959	0.251049
20	6	0	3.386190	-0.839118	-0.310948
21	6	0	3.251126	1.605673	-0.321264
22	1	0	1.378180	2.509486	0.239967
23	1	0	3.944958	-1.756700	-0.471406
24	6	0	3.972931	0.407653	-0.525574
25	1	0	3.742360	2.557127	-0.501923
26	1	0	5.005461	0.458921	-0.857832
27	8	0	-1.874268	-1.328967	-1.150146
28	1	0	-0.946171	-1.561922	-0.405879

Rotational constants (GHZ): 1.2766750 0.3760880 0.3169983
E[B3LYP/6-31++G(d,p)] = -686.9141661 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.0754240 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2537531 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2606244 a.u.
ZPVE = 584.1834 kJ mol^{-1}

Table S30. B3LYP/6-31++G(d,p) optimized structure of **TS8**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.676800	1.000280	0.162344
2	1	0	2.685484	-2.589916	-0.265162
3	1	0	4.048076	0.589373	-0.691789
4	1	0	4.262253	0.657428	0.920586
5	6	0	2.288293	0.569376	0.364094
6	1	0	1.940191	0.987093	1.314908
7	6	0	1.403964	1.198139	-0.764311
8	6	0	2.122240	-0.933151	0.476358
9	1	0	1.788959	2.211555	-0.920428
10	1	0	1.572797	0.646874	-1.699229
11	6	0	-0.061888	1.262604	-0.430560
12	8	0	2.911515	-1.654950	-0.387156
13	6	0	-0.744158	2.393358	-0.026559
14	6	0	-1.001582	0.184375	-0.366667
15	1	0	-0.393247	3.412259	0.062289
16	7	0	-2.045146	2.064070	0.297209

17	6	0	-2.225201	0.705173	0.117540
18	6	0	-0.870842	-1.238838	-0.586993
19	1	0	-2.743397	2.708273	0.631963
20	6	0	-3.354229	-0.094838	0.349204
21	6	0	-2.059075	-2.020847	-0.415914
22	1	0	-0.160089	-1.574305	-1.348778
23	1	0	-4.285191	0.327993	0.714960
24	6	0	-3.239949	-1.468182	0.079957
25	1	0	-2.029003	-3.079321	-0.658484
26	1	0	-4.102602	-2.109130	0.237669
27	8	0	1.132404	-1.527321	1.047846
28	1	0	0.097406	-1.523481	0.422203

Rotational constants (GHZ): 1.0511623 0.4604083 0.3441143

E[B3LYP/6-31++G(d,p)] = -686.9145929 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.0761593 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2552190 a.u.
E[ROMP2/6-311++G(2d,p)] = convergence failed
ZPVE = 584.1915 kJ mol^{-1}

Table S31. B3LYP/6-31++G(d,p) optimized structure of **TS9**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.080475	1.412788	0.917064
2	1	0	-2.057799	0.891149	1.809554
3	1	0	-2.786848	2.154906	0.987967
4	1	0	-1.054366	1.883872	0.720078
5	6	0	-2.366310	0.442877	-0.192613
6	1	0	-3.385040	0.620585	-0.552492
7	6	0	-1.361932	0.704299	-1.399878
8	6	0	-2.333577	-0.942003	0.406182
9	1	0	-1.420318	-0.165639	-2.058290
10	1	0	-1.767438	1.559228	-1.952227
11	6	0	0.017612	0.981436	-0.924653
12	8	0	-2.228508	-1.160574	1.607500
13	6	0	0.356211	2.219239	-0.273402
14	6	0	1.006416	0.020999	-0.570238
15	1	0	0.129337	3.202502	-0.684344
16	7	0	1.664601	2.033685	0.246219
17	6	0	2.026495	0.707764	0.165135
18	6	0	1.138542	-1.372868	-0.773566
19	1	0	2.128373	2.701562	0.841110
20	6	0	3.142822	0.045457	0.681934
21	6	0	2.263831	-2.029602	-0.268841
22	1	0	0.385739	-1.922003	-1.332059
23	1	0	3.904486	0.579725	1.243285
24	6	0	3.252205	-1.334527	0.448271
25	1	0	2.376440	-3.098406	-0.429021
26	1	0	4.113614	-1.872636	0.832884
27	8	0	-2.524292	-1.908918	-0.520222

28	1	0	-2.486554	-2.762654	-0.057647

Rotational constants (GHZ): 0.9307103 0.4884381 0.3859259
E[B3LYP/6-31++G(d,p)] = -686.9079188 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.0699082 a.u.
E[PMP2/6-311++G(2d,p)] = -685.246416 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2549728 a.u.
ZPVE = 585.3615 kJ mol^{-1}

Table S32. B3LYP/6-31++G(d,p) optimized structure of **TS11**
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.575988	-0.894793	1.284576
2	1	0	-3.082444	-1.969896	0.307352
3	1	0	-1.697782	-0.898119	2.294897
4	1	0	-0.578005	-0.849484	1.094935
5	6	0	-2.283132	0.204720	0.660005
6	1	0	-2.186624	1.213959	1.056718
7	6	0	-1.006680	0.635992	-1.026938
8	6	0	-3.526542	-0.172173	0.179605
9	1	0	-1.145335	-0.288763	-1.581662
10	1	0	-1.601121	1.464784	-1.401006
11	6	0	0.320684	0.929165	-0.559392
12	8	0	-3.829054	-1.467003	-0.085191
13	6	0	0.803330	2.151679	-0.098851
14	6	0	1.423858	-0.009867	-0.390421
15	1	0	0.310684	3.112987	-0.062555
16	7	0	2.114803	2.014937	0.330479
17	6	0	2.520964	0.706545	0.162525
18	6	0	1.584133	-1.376907	-0.676244
19	1	0	2.689396	2.762727	0.683864
20	6	0	3.749726	0.096085	0.440270
21	6	0	2.803729	-1.991191	-0.402798
22	1	0	0.768290	-1.949161	-1.109230
23	1	0	4.578105	0.658320	0.862664
24	6	0	3.875380	-1.260693	0.152458
25	1	0	2.935522	-3.046681	-0.621526
26	1	0	4.816374	-1.763403	0.355688
27	8	0	-4.421738	0.717576	-0.307315
28	1	0	-5.165143	0.226999	-0.686794

Rotational constants (GHZ): 1.2712809 0.3086384 0.2684650
E[B3LYP/6-31++G(d,p)] = -686.9186897 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.0814172 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2621019 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2611363 a.u.
ZPVE = 589.5284 kJ mol^{-1}

Table S33. B3LYP/6-31++G(d,p) optimized structure of **TS10**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.796152	-0.397204	2.027343
2	1	0	4.229732	0.175153	-1.428395
3	1	0	3.526955	0.309530	2.024696
4	1	0	3.242201	-1.311486	2.078772
5	6	0	1.952268	-0.279693	0.825716
6	1	0	1.233184	-1.104095	0.856305
7	6	0	1.199723	1.029029	0.818653
8	6	0	2.714647	-0.452821	-0.489143
9	1	0	0.522714	1.148159	1.660864
10	1	0	1.786038	1.916809	0.584961
11	6	0	-0.271406	1.100185	-0.812497
12	8	0	3.814480	0.343886	-0.565644
13	6	0	-0.990261	2.287589	-0.581558
14	6	0	-1.203398	0.016997	-0.495186
15	1	0	-0.689876	3.314521	-0.728385
16	7	0	-2.188092	1.983597	0.039450
17	6	0	-2.358026	0.607401	0.079600
18	6	0	-1.141809	-1.376835	-0.627017
19	1	0	-2.869820	2.660666	0.342523
20	6	0	-3.433148	-0.155024	0.546516
21	6	0	-2.216375	-2.145198	-0.176317
22	1	0	-0.272104	-1.844645	-1.079118
23	1	0	-4.309039	0.309952	0.990320
24	6	0	-3.344570	-1.540067	0.410216
25	1	0	-2.184228	-3.225783	-0.278662
26	1	0	-4.164949	-2.161470	0.757249
27	8	0	2.403105	-1.201761	-1.394592
28	1	0	0.506222	1.021563	-1.560696

Rotational constants (GHZ): 1.0276953 0.3729061 0.3304472

E[B3LYP/6-31++G(d,p)] = -686.9290121 a.u.
E[B3LYP/6-311++G(2d,p)] = -687.09188741 a.u.
E[PMP2/6-311++G(2d,p)] = -685.2227686 a.u.
E[ROMP2/6-311++G(2d,p)] = -685.2739494 a.u.
ZPVE = 589.7227 kJ mol^{-1}

Table S34. Excitation Energies of $\mathbf{1}^+$ (eV)**.**

State	Singlet	Triplet
X	0.0	3.47
A	3.92	3.95
B	4.18	4.10
C	4.38	4.23
D	4.63	4.81
E	4.70	4.82
F	4.82	5.36
G	5.30	5.49
H	5.39	5.64
I	5.61	6.06
J	5.72	6.10