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"Unexpected Conformational Properties of 1-Trifluormethyl-1-Silacyclohexane, $C_5H_{10}SiHCF_3$: Gas Electron Diffraction, Low Temperature NMR, and Quantum Chemical Calculations[§]"

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[§] *Conformations of Silicon-Containing Rings. Part 6. For Part 5 see ref. [1]*

*Structure **5a**:*

*B3LYP/6-31G** geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.139578	0.000000	1.049141
2	6	0	-0.938990	1.510660	0.716146
3	6	0	-0.938991	-1.510659	0.716146
4	6	0	-1.820507	1.296549	-0.538140
5	6	0	-1.820508	-1.296549	-0.538139
6	6	0	-2.652286	-0.000001	-0.505965
7	1	0	0.777360	0.000000	2.391955
8	6	0	1.620330	0.000000	-0.195213
9	9	0	1.207288	0.000000	-1.497008
10	9	0	2.417506	-1.091124	-0.045027
11	9	0	2.417506	1.091124	-0.045028
12	1	0	-0.332199	2.417790	0.615642
13	1	0	-1.579486	1.665946	1.595561
14	1	0	-0.332200	-2.417790	0.615643
15	1	0	-1.579486	-1.665945	1.595562
16	1	0	-1.182545	1.286052	-1.430898
17	1	0	-2.496618	2.152675	-0.654767
18	1	0	-1.182546	-1.286051	-1.430898
19	1	0	-2.496618	-2.152675	-0.654767
20	1	0	-3.333100	-0.000001	-1.365626
21	1	0	-3.291652	-0.000001	0.389169

SCF Done: E(RBLYP) = -824.317794616 A.U. after 13 cycles

No. of imaginary frequencies: 0

Zero-point correction= 0.164750 (Hartree/Particle)

Thermal correction to Energy= 0.175431

Thermal correction to Enthalpy= 0.176375

Thermal correction to Gibbs Free Energy= 0.127794

*Structure **5a**:*

*MP2/6-31G** geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.133905	0.000005	1.063635
2	6	0	0.935609	-1.503920	0.723082
3	6	0	0.935601	1.503934	0.723073
4	6	0	1.782134	-1.287075	-0.544734
5	6	0	1.782127	1.287085	-0.544742
6	6	0	2.613301	-0.000012	-0.515029
7	1	0	-0.780803	0.000007	2.391213
8	6	0	-1.594572	-0.000003	-0.193105
9	9	0	-1.167313	-0.000006	-1.493514
10	9	0	-2.395487	1.093332	-0.053254
11	9	0	-2.395481	-1.093342	-0.053247
12	1	0	0.330412	-2.408371	0.633919
13	1	0	1.599472	-1.657184	1.579405
14	1	0	0.330398	2.408381	0.633904
15	1	0	1.599463	1.657207	1.579395
16	1	0	1.128463	-1.262036	-1.419870
17	1	0	2.450563	-2.140354	-0.681386
18	1	0	1.128458	1.262048	-1.419878
19	1	0	2.450565	2.140358	-0.681389
20	1	0	3.287685	-0.000018	-1.374288
21	1	0	3.249311	-0.000013	0.376941

SCF Done: E(RHF) = -820.886056818 A.U. after 12 cycles

E2 = -0.1445532709D+01 EUMP2 = -0.82233158952622D+03

No. of imaginary frequencies: 0

Zero-point correction= 0.169420 (Hartree/Particle)

Thermal correction to Energy= 0.179892

Thermal correction to Enthalpy= 0.180836

Thermal correction to Gibbs Free Energy= 0.132850

*Structure **5a**:*

B3LYP/6-311G geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.172542	0.013780	1.508491
2	6	0	-1.172542	-1.518558	1.295774
3	6	0	-1.868874	-1.971938	0.000000
4	6	0	-1.172542	-1.518558	-1.295774
5	6	0	-1.172542	0.013780	-1.508491
6	14	0	-0.503999	0.919392	-0.000000
7	1	0	-1.928711	-3.065527	0.000000
8	1	0	-0.140345	-1.886398	1.292311
9	1	0	-1.660587	-1.999025	2.150853
10	1	0	-2.200713	0.361191	1.674649
11	1	0	-0.616725	0.279904	2.413226
12	1	0	-0.140345	-1.886398	-1.292311
13	1	0	-1.660587	-1.999025	-2.150853
14	1	0	-0.616725	0.279904	-2.413226
15	1	0	-2.200713	0.361191	-1.674649
16	1	0	-0.788538	2.376368	-0.000000
17	1	0	-2.907566	-1.613579	0.000000
18	6	0	1.431947	0.807646	-0.000000
19	9	0	1.983765	1.404569	-1.090225
20	9	0	1.983765	1.404569	1.090225
21	9	0	1.885818	-0.479916	-0.000000

SCF Done: E(RB+HF-LYP) = -824.472249791 A.U. after 13 cycles

No. of imaginary frequencies: 0

Zero-point correction= 0.164224 (Hartree/Particle)

Thermal correction to Energy= 0.174931

Thermal correction to Enthalpy= 0.175875

Thermal correction to Gibbs Free Energy= 0.127250

*Structure **5a**:*

CBS-QB3 calculation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.934421	-1.504824	0.705352
2	6	0	-1.836294	-1.295614	-0.535443
3	6	0	-2.667441	0.000000	-0.492456
4	6	0	-1.836294	1.295614	-0.535444
5	6	0	-0.934421	1.504824	0.705352
6	14	0	0.136142	-0.000000	1.038321
7	1	0	-3.358065	0.000000	-1.341927
8	1	0	-1.216081	-1.288822	-1.438522
9	1	0	-2.512860	-2.150855	-0.635602
10	1	0	-1.561205	-1.662140	1.592806
11	1	0	-0.326017	-2.408088	0.598095
12	1	0	-1.216081	1.288822	-1.438522
13	1	0	-2.512860	2.150855	-0.635602
14	1	0	-0.326017	2.408088	0.598095
15	1	0	-1.561205	1.662140	1.592806
16	1	0	0.769716	0.000000	2.376579
17	1	0	-3.293942	0.000000	0.409816
18	6	0	1.625763	-0.000000	-0.192401
19	9	0	2.423463	1.090657	-0.035794
20	9	0	2.423463	-1.090657	-0.035794
21	9	0	1.231661	-0.000000	-1.500000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.162058	E(Thermal)=	0.172860
E(SCF)=	-821.077728	DE(MP2)=	-1.867302
DE(CBS)=	-0.193733	DE(MP34)=	-0.081785
DE(CCSD)=	-0.043443	DE(Int)=	0.060218
DE(Empirical)=	-0.096874		
CBS-QB3 (0 K)=	-823.138589	CBS-QB3 Energy=	-823.127788
CBS-QB3 Enthalpy=	-823.126843	CBS-QB3 Free Energy=	-823.175641

*Structure **5a**:*

B3LYP/6-311G PCM geometry optimization, CH_2Cl_2 solvent*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.939254	-1.510758	-0.695273
2	6	0	1.849390	-1.295851	0.537555
3	6	0	2.678868	-0.000049	0.487074
4	6	0	1.849402	1.295756	0.537682
5	6	0	0.939465	1.510795	-0.695265
6	14	0	-0.124858	0.000115	-1.040030
7	1	0	3.377806	-0.000108	1.330758
8	1	0	1.239240	-1.292742	1.448583
9	1	0	2.527982	-2.150967	0.632688
10	1	0	1.561032	-1.677027	-1.585109
11	1	0	0.331855	-2.414709	-0.579045
12	1	0	1.238990	1.292581	1.448574
13	1	0	2.527974	2.150867	0.633028
14	1	0	0.332166	2.414807	-0.579125
15	1	0	1.561320	1.676851	-1.585077
16	1	0	-0.771165	-0.000175	-2.375748
17	1	0	3.298146	0.000015	-0.420532
18	6	0	-1.632615	0.000021	0.187333
19	9	0	-2.436385	1.090787	0.030566
20	9	0	-2.438923	-1.088380	0.027193
21	9	0	-1.260238	-0.002463	1.501885

SCF Done: E(RB+HF-LYP) = -824.475811029 A.U. after 1 cycles
No. of imaginary frequencies: 0
Zero-point correction= 0.163377 (Hartree/Particle)
Thermal correction to Energy= 0.174134
Thermal correction to Enthalpy= 0.175078
Thermal correction to Gibbs Free Energy= 0.126365

*Structure **5a**:*

B3LYP/6-311G PCM geometry optimization, $CHCl_3$ solvent*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.939839	1.510895	-0.695453
2	6	0	-1.849735	1.295407	0.537407
3	6	0	-2.678527	-0.000819	0.486983
4	6	0	-1.848371	-1.296193	0.536872
5	6	0	-0.938634	-1.510379	-0.696346
6	14	0	0.126169	0.000761	-1.039212
7	1	0	-3.377067	-0.001346	1.330895
8	1	0	-1.239218	1.292384	1.448059
9	1	0	-2.528619	2.150154	0.633117
10	1	0	-1.561528	1.677892	-1.585130
11	1	0	-0.332616	2.414777	-0.578607
12	1	0	-1.237463	-1.292761	1.447267
13	1	0	-2.526324	-2.151680	0.632568
14	1	0	-0.330625	-2.413800	-0.580063
15	1	0	-1.560395	-1.677464	-1.585949
16	1	0	0.769975	0.001391	-2.376335
17	1	0	-3.298627	-0.000966	-0.420077
18	6	0	1.633028	0.000199	0.188009
19	9	0	2.438081	-1.088236	0.026518
20	9	0	2.435534	1.091151	0.031669
21	9	0	1.258453	-0.003348	1.501634

SCF Done: E(RB+HF-LYP) = -824.475225697 A.U. after 1 cycles
Zero-point correction= 0.163525 (Hartree/Particle)
Thermal correction to Energy= 0.174273
Thermal correction to Enthalpy= 0.175217
Thermal correction to Gibbs Free Energy= 0.126514

*Structure **5a**:*

B3LYP/6-311G IPCM calculation, CH_2Cl_2 solvent (e = 8.93)*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.939254	-1.510758	-0.695273
2	6	0	1.849390	-1.295851	0.537555
3	6	0	2.678868	-0.000049	0.487074
4	6	0	1.849402	1.295756	0.537682
5	6	0	0.939465	1.510795	-0.695265
6	14	0	-0.124858	0.000115	-1.040030
7	1	0	3.377806	-0.000108	1.330758
8	1	0	1.239240	-1.292742	1.448583
9	1	0	2.527982	-2.150967	0.632688
10	1	0	1.561032	-1.677027	-1.585109
11	1	0	0.331855	-2.414709	-0.579045
12	1	0	1.238990	1.292581	1.448574
13	1	0	2.527974	2.150867	0.633028
14	1	0	0.332166	2.414807	-0.579125
15	1	0	1.561320	1.676851	-1.585077
16	1	0	-0.771165	-0.000175	-2.375748
17	1	0	3.298146	0.000015	-0.420532
18	6	0	-1.632615	0.000021	0.187333
19	9	0	-2.436385	1.090787	0.030566
20	9	0	-2.438923	-1.088380	0.027193
21	9	0	-1.260238	-0.002463	1.501885

SCF Done: E(RB+HF-LYP) = -824.475929164 A.U. after 9 cycles

*Structure **5a**:*

B3LYP/6-311G IPCM calculation, $CHCl_3$ solvent (e = 4.9)*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.939839	1.510895	-0.695453
2	6	0	-1.849735	1.295407	0.537407
3	6	0	-2.678527	-0.000819	0.486983
4	6	0	-1.848371	-1.296193	0.536872
5	6	0	-0.938634	-1.510379	-0.696346
6	14	0	0.126169	0.000761	-1.039212
7	1	0	-3.377067	-0.001346	1.330895
8	1	0	-1.239218	1.292384	1.448059
9	1	0	-2.528619	2.150154	0.633117
10	1	0	-1.561528	1.677892	-1.585130
11	1	0	-0.332616	2.414777	-0.578607
12	1	0	-1.237463	-1.292761	1.447267
13	1	0	-2.526324	-2.151680	0.632568
14	1	0	-0.330625	-2.413800	-0.580063
15	1	0	-1.560395	-1.677464	-1.585949
16	1	0	0.769975	0.001391	-2.376335
17	1	0	-3.298627	-0.000966	-0.420077
18	6	0	1.633028	0.000199	0.188009
19	9	0	2.438081	-1.088236	0.026518
20	9	0	2.435534	1.091151	0.031669
21	9	0	1.258453	-0.003348	1.501634

SCF Done: E(RB+HF-LYP) = -824.475295136 A.U. after 9 cycles

*Structure **5e**:*

*B3LYP/6-31G** geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.076672	0.000001	-0.605568
2	6	0	0.861479	1.508271	0.026442
3	6	0	0.861482	-1.508269	0.026440
4	6	0	2.387424	1.296012	-0.123602
5	6	0	2.387426	-1.296007	-0.123604
6	6	0	2.906871	-0.000005	0.526785
7	1	0	-0.210849	0.000002	-2.087505
8	6	0	-1.887869	-0.000001	0.065227
9	9	0	-1.926867	-0.000002	1.427254
10	9	0	-2.587947	-1.091293	-0.343909
11	9	0	-2.587948	1.091291	-0.343907
12	1	0	0.614190	1.646857	1.087523
13	1	0	0.544473	2.422411	-0.487251
14	1	0	0.614193	-1.646856	1.087521
15	1	0	0.544476	-2.422409	-0.487254
16	1	0	2.915828	2.152459	0.313398
17	1	0	2.655815	1.289330	-1.189522
18	1	0	2.915831	-2.152457	0.313389
19	1	0	2.655816	-1.289319	-1.189524
20	1	0	2.645009	-0.000008	1.594650
21	1	0	4.002616	-0.000006	0.481455

SCF Done: E(RBLYP) = -824.317047920 A.U. after 7 cycles
No. of imaginary frequencies: 0
Zero-point correction= 0.164487 (Hartree/Particle)
Thermal correction to Energy= 0.175307
Thermal correction to Enthalpy= 0.176251
Thermal correction to Gibbs Free Energy= 0.127058

*Structure **5e**:*

*MP2/6-31G** geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.069961	0.000001	-0.604230
2	6	0	-0.854921	-1.496641	0.046316
3	6	0	-0.854918	1.496644	0.046319
4	6	0	-2.369757	-1.286660	-0.132195
5	6	0	-2.369754	1.286667	-0.132192
6	6	0	-2.890821	-0.000007	0.516226
7	1	0	0.180885	0.000003	-2.078596
8	6	0	1.875142	-0.000001	0.057961
9	9	0	1.907579	-0.000002	1.423237
10	9	0	2.579873	1.093332	-0.347048
11	9	0	2.579871	-1.093335	-0.347050
12	1	0	-0.628967	-1.608621	1.110694
13	1	0	-0.531959	-2.417647	-0.442079
14	1	0	-0.628964	1.608622	1.110697
15	1	0	-0.531954	2.417651	-0.442075
16	1	0	-2.905780	-2.141036	0.287342
17	1	0	-2.616798	-1.265808	-1.198632
18	1	0	-2.905776	2.141039	0.287355
19	1	0	-2.616797	1.265822	-1.198630
20	1	0	-2.627067	-0.000010	1.578857
21	1	0	-3.982021	-0.000008	0.467424

SCF Done: E(RHF) = -820.886028483 A.U. after 7 cycles
E2 = -0.1444434231D+01 EUMP2 = -0.82233046271358D+03
No. of imaginary frequencies: 0
Zero-point correction= 0.169213 (Hartree/Particle)
Thermal correction to Energy= 0.179819
Thermal correction to Enthalpy= 0.180764
Thermal correction to Gibbs Free Energy= 0.132096

*Structure **5e**:*

B3LYP/6-311G geometry optimization*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.862994	-1.505009	0.033823
2	6	0	2.388120	-1.295640	-0.123928
3	6	0	2.913139	0.000239	0.519627
4	6	0	2.387710	1.295947	-0.123943
5	6	0	0.862509	1.504723	0.033705
6	14	0	-0.070694	-0.000320	-0.601525
7	1	0	2.665267	0.000205	1.589365
8	1	0	2.915324	-2.151112	0.312178
9	1	0	2.652053	-1.295869	-1.189493
10	1	0	0.543897	-2.419559	-0.475032
11	1	0	0.621235	-1.644121	1.094630
12	1	0	2.914585	2.151599	0.312208
13	1	0	2.651712	1.296286	-1.189492
14	1	0	0.620639	1.643861	1.094488
15	1	0	0.543013	2.419080	-0.475244
16	1	0	-0.197058	-0.000417	-2.081909
17	1	0	4.007024	0.000402	0.464047
18	6	0	-1.889843	-0.000094	0.061556
19	9	0	-1.938773	-0.002932	1.423735
20	9	0	-2.590204	1.091945	-0.345068
21	9	0	-2.592774	-1.088665	-0.349714

SCF Done: E(RB+HF-LYP) = -824.471675812 A.U. after 13 cycles
No. of imaginary frequencies: 0
Zero-point correction= 0.164057 (Hartree/Particle)
Thermal correction to Energy= 0.174869
Thermal correction to Enthalpy= 0.175813
Thermal correction to Gibbs Free Energy= 0.126612

*Structure **5e**:*

CBS-QB3 calculation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.857755	-1.500670	0.041468
2	6	0	2.383427	-1.296197	-0.127090
3	6	0	2.914823	0.000046	0.511835
4	6	0	2.383340	1.296241	-0.127112
5	6	0	0.857661	1.500620	0.041469
6	14	0	-0.070492	-0.000054	-0.595357
7	1	0	2.673539	0.000048	1.582800
8	1	0	2.911571	-2.151317	0.307602
9	1	0	2.638659	-1.295773	-1.194530
10	1	0	0.531028	-2.415466	-0.461379
11	1	0	0.620464	-1.627118	1.104708
12	1	0	2.911449	2.151407	0.307534
13	1	0	2.638541	1.295797	-1.194561
14	1	0	0.620393	1.627103	1.104714
15	1	0	0.530840	2.415372	-0.461392
16	1	0	-0.192453	-0.000033	-2.072189
17	1	0	4.007699	0.000081	0.445581
18	6	0	-1.885185	-0.000019	0.060123
19	9	0	-1.938855	-0.002852	1.422222
20	9	0	-2.583851	1.092226	-0.349804
21	9	0	-2.585712	-1.089315	-0.354425

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.161869	E(Thermal)=	0.172784
E(SCF)=	-821.077655	DE(MP2)=	-1.866327
DE(CBS)=	-0.193767	DE(MP34)=	-0.081820
DE(CCSD)=	-0.043365	DE(Int)=	0.060212
DE(Empirical)=	-0.096882		
CBS-QB3 (0 K)=	-823.137736	CBS-QB3 Energy=	-823.126820
CBS-QB3 Enthalpy=	-823.125876	CBS-QB3 Free Energy=	-823.175206

*Structure **5e**:*

B3LYP/6-311G PCM geometry optimization, CH_2Cl_2 solvent*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863558	-1.507323	0.033169
2	6	0	2.389605	-1.295354	-0.122820
3	6	0	2.911847	0.000410	0.523336
4	6	0	2.388908	1.295880	-0.122832
5	6	0	0.862712	1.506818	0.032981
6	14	0	-0.061369	-0.000539	-0.602994
7	1	0	2.659496	0.000346	1.592349
8	1	0	2.915010	-2.151408	0.314924
9	1	0	2.654418	-1.294108	-1.188359
10	1	0	0.545496	-2.420746	-0.479457
11	1	0	0.622083	-1.646124	1.094709
12	1	0	2.913745	2.152269	0.314940
13	1	0	2.653776	1.294768	-1.188359
14	1	0	0.621194	1.645660	1.094511
15	1	0	0.543930	2.419894	-0.479809
16	1	0	-0.211918	-0.000551	-2.080586
17	1	0	4.006171	0.000693	0.469869
18	6	0	-1.885241	-0.000205	0.060694
19	9	0	-1.949179	-0.007546	1.424038
20	9	0	-2.592052	1.093775	-0.342087
21	9	0	-2.597944	-1.085619	-0.354171

SCF Done: E(RB+HF-LYP) = -824.475335133 A.U. after 1 cycles
No. of imaginary frequencies: 0
Zero-point correction= 0.163192 (Hartree/Particle)
Thermal correction to Energy= 0.174049
Thermal correction to Enthalpy= 0.174993
Thermal correction to Gibbs Free Energy= 0.125795

*Structure **5e**:*

B3LYP/6-311G PCM geometry optimization, $CHCl_3$ solvent*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863926	-1.507304	0.034752
2	6	0	2.389781	-1.295217	-0.123815
3	6	0	2.912813	0.000597	0.521609
4	6	0	2.388737	1.296087	-0.123585
5	6	0	0.862652	1.506553	0.034237
6	14	0	-0.062443	-0.000871	-0.600752
7	1	0	2.661912	0.000327	1.590945
8	1	0	2.916437	-2.151158	0.312600
9	1	0	2.652794	-1.293872	-1.189815
10	1	0	0.545305	-2.421175	-0.476596
11	1	0	0.624206	-1.646007	1.096596
12	1	0	2.914369	2.152427	0.313281
13	1	0	2.652205	1.295227	-1.189473
14	1	0	0.622238	1.645627	1.095895
15	1	0	0.543091	2.419743	-0.477743
16	1	0	-0.209216	-0.001045	-2.078956
17	1	0	4.007055	0.001061	0.467004
18	6	0	-1.886307	-0.000257	0.060503
19	9	0	-1.949826	-0.003984	1.423634
20	9	0	-2.592069	1.092274	-0.346240
21	9	0	-2.596528	-1.087370	-0.352441

SCF Done: E(RB+HF-LYP) = -824.474777291 A.U. after 11 cycles
No. of imaginary frequencies: 0
Zero-point correction= 0.163336 (Hartree/Particle)
Thermal correction to Energy= 0.174181
Thermal correction to Enthalpy= 0.175125
Thermal correction to Gibbs Free Energy= 0.125950

*Structure **5e**:*

B3LYP/6-311G IPCM calculation, CH_2Cl_2 solvent (e = 8.93)*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863558	-1.507323	0.033169
2	6	0	2.389605	-1.295354	-0.122820
3	6	0	2.911847	0.000410	0.523336
4	6	0	2.388908	1.295880	-0.122832
5	6	0	0.862712	1.506818	0.032981
6	14	0	-0.061369	-0.000539	-0.602994
7	1	0	2.659496	0.000346	1.592349
8	1	0	2.915010	-2.151408	0.314924
9	1	0	2.654418	-1.294108	-1.188359
10	1	0	0.545496	-2.420746	-0.479457
11	1	0	0.622083	-1.646124	1.094709
12	1	0	2.913745	2.152269	0.314940
13	1	0	2.653776	1.294768	-1.188359
14	1	0	0.621194	1.645660	1.094511
15	1	0	0.543930	2.419894	-0.479809
16	1	0	-0.211918	-0.000551	-2.080586
17	1	0	4.006171	0.000693	0.469869
18	6	0	-1.885241	-0.000205	0.060694
19	9	0	-1.949179	-0.007546	1.424038
20	9	0	-2.592052	1.093775	-0.342087
21	9	0	-2.597944	-1.085619	-0.354171

SCF Done: E(RB+HF-LYP) = -824.476775375 A.U. after 7 cycles

*Structure **5e**:*

B3LYP/6-311G IPCM calculation, $CHCl_3$ solvent (e = 4.9)*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863926	-1.507304	0.034752
2	6	0	2.389781	-1.295217	-0.123815
3	6	0	2.912813	0.000597	0.521609
4	6	0	2.388737	1.296087	-0.123585
5	6	0	0.862652	1.506553	0.034237
6	14	0	-0.062443	-0.000871	-0.600752
7	1	0	2.661912	0.000327	1.590945
8	1	0	2.916437	-2.151158	0.312600
9	1	0	2.652794	-1.293872	-1.189815
10	1	0	0.545305	-2.421175	-0.476596
11	1	0	0.624206	-1.646007	1.096596
12	1	0	2.914369	2.152427	0.313281
13	1	0	2.652205	1.295227	-1.189473
14	1	0	0.622238	1.645627	1.095895
15	1	0	0.543091	2.419743	-0.477743
16	1	0	-0.209216	-0.001045	-2.078956
17	1	0	4.007055	0.001061	0.467004
18	6	0	-1.886307	-0.000257	0.060503
19	9	0	-1.949826	-0.003984	1.423634
20	9	0	-2.592069	1.092274	-0.346240
21	9	0	-2.596528	-1.087370	-0.352441

SCF Done: E(RB+HF-LYP) = -824.475936712 A.U. after 7 cycles

*Structure **5c**:*

CBS-QB3 calculation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.879373	-1.340111	-0.775296
2	6	0	1.782750	-1.351065	0.479292
3	6	0	2.862689	-0.242110	0.496234
4	6	0	2.441986	1.121916	-0.104157
5	6	0	0.963377	1.498189	0.151831
6	14	0	-0.101188	0.266970	-0.791379
7	1	0	3.179992	-0.095909	1.533962
8	1	0	1.147953	-1.253648	1.366595
9	1	0	2.277165	-2.322415	0.578359
10	1	0	1.481281	-1.413337	-1.688263
11	1	0	0.210134	-2.205546	-0.778799
12	1	0	3.103242	1.899092	0.291090
13	1	0	2.621278	1.111245	-1.186478
14	1	0	0.735417	1.454516	1.222506
15	1	0	0.762484	2.523431	-0.169985
16	1	0	-0.470552	0.732191	-2.148121
17	1	0	3.749182	-0.591352	-0.043612
18	6	0	-1.783171	0.006243	0.118433
19	9	0	-1.613544	-0.459645	1.389637
20	9	0	-2.497299	1.158563	0.225094
21	9	0	-2.585043	-0.891610	-0.514284

No. of imaginary frequencies: 0

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.161951	E(Thermal)=	0.172927
E(SCF)=	-821.071248	DE(MP2)=	-1.867674
DE(CBS)=	-0.193799	DE(MP34)=	-0.081756
DE(CCSD)=	-0.043479	DE(Int)=	0.060235
DE(Empirical)=	-0.096864		
CBS-QB3 (0 K)=	-823.132634	CBS-QB3 Energy=	-823.121658
CBS-QB3 Enthalpy=	-823.120714	CBS-QB3 Free Energy=	-823.170241

*Structure **5a–5b**:*

*B3LYP/6-311+G** STQN(Path) calculation input file*

```
#b3lyp/6-311+G** opt(qst3,path=11)

a

0 1
             6                  -0.940304   -1.511059    0.716595
             6                  -1.821426   -1.296792   -0.538348
             6                  -2.653436    0.000000   -0.506116
             6                  -1.821426    1.296792   -0.538348
             6                  -0.940304    1.511059    0.716595
            14                   0.139502   -0.000000    1.047671
             1                  -3.334360    0.000000   -1.366885
             1                  -1.183036   -1.286704   -1.431774
             1                  -2.498442   -2.153476   -0.654572
             1                  -1.582637   -1.666120    1.595868
             1                  -0.334937   -2.420264    0.615337
             1                  -1.183035    1.286704   -1.431774
             1                  -2.498442    2.153476   -0.654572
             1                  -0.334937    2.420264    0.615337
             1                  -1.582637    1.666120    1.595868
             1                   0.778015   -0.000000    2.391508
             1                  -3.293283    0.000000    0.389734
             6                   1.621413   -0.000000   -0.195084
             9                   2.418420    1.091044   -0.043632
             9                   2.418420   -1.091044   -0.043632
             9                   1.210671   -0.000000   -1.497540

b

0 1
             6                   0.836301   -1.550803   -0.177607
             6                   2.172877   -1.233229    0.538594
             6                   2.966864   -0.123193   -0.177224
             6                   2.431058    1.311917    0.062467
             6                   0.887397    1.444515    0.212238
            14                  -0.061057    0.054875   -0.638441
             1                   4.019319   -0.157058    0.129613
             1                   1.979080   -0.935179    1.578066
             1                   2.781242   -2.144885    0.592819
             1                   1.037092   -2.124798   -1.091394
             1                   0.199671   -2.185719    0.450798
             1                   2.899644    1.718872    0.967487
             1                   2.769488    1.948721   -0.763274
             1                   0.613457    1.373413    1.274064
             1                   0.551516    2.434604   -0.114449
             1                  -0.216132    0.238798   -2.107557
             1                   2.964610   -0.343503   -1.255590
```

```
             6                   -1.866970    0.019950    0.043835
             9                   -2.543654    1.171598   -0.207357
             9                   -2.601022   -0.991610   -0.492097
             9                   -1.889696   -0.158482    1.395429

ts

0 1
             6                    0.836747   -1.562983   -0.243368
             6                    2.140747   -1.254943    0.529583
             6                    2.947269   -0.110174   -0.111938
             6                    2.399548    1.296748    0.204619
             6                    0.865372    1.514690    0.001203
            14                   -0.074395    0.031794   -0.706265
             1                    3.989969   -0.153059    0.227358
             1                    1.905461   -0.990752    1.570147
             1                    2.756547   -2.162061    0.577588
             1                    1.079978   -2.101853   -1.168513
             1                    0.185794   -2.229319    0.335779
             1                    2.645357    1.525667    1.249255
             1                    2.952194    2.025698   -0.399504
             1                    0.395822    1.745992    0.965768
             1                    0.681332    2.393092   -0.627413
             1                   -0.318896    0.140652   -2.170644
             1                    2.979861   -0.266100   -1.201688
             6                   -1.840642    0.015264    0.073996
             9                   -2.544664    1.145187   -0.201498
             9                   -2.590072   -1.031153   -0.364440
             9                   -1.788169   -0.087888    1.433161
```

Converged Path:

```
Min E( 1) =  -824.499043908
    E( 2) =  -824.498043541
    E( 3) =  -824.495773739
    E( 4) =  -824.493337717
    E( 5) =  -824.491715874
TS  E( 6) =  -824.491217539
    E( 7) =  -824.491262868
    E( 8) =  -824.491368216
    E( 9) =  -824.491498445
    E(10) =  -824.491615607
Min E(11) =  -824.491659738
```

*Structure **5b–5c**:*

*B3LYP/6-311+G** STQN(Path) calculation input file*

```
#b3lyp/6-311+G** opt(qst3,path=11)

b

0 1
             6                    0.836313   -1.550683   -0.178921
             6                    2.171936   -1.233265    0.539065
             6                    2.967061   -0.123521   -0.175939
             6                    2.431087    1.311814    0.062303
             6                    0.887414    1.444591    0.211574
            14                   -0.061218    0.055071   -0.639116
             1                    4.019043   -0.157394    0.132505
             1                    1.976810   -0.935055    1.578241
             1                    2.780077   -2.145019    0.594202
             1                    1.038460   -2.123571   -1.093111
             1                    0.199262   -2.186612    0.448030
             1                    2.899407    1.719661    0.967055
             1                    2.769706    1.947880   -0.763930
             1                    0.613159    1.373685    1.273331
             1                    0.551804    2.434703   -0.115329
             1                   -0.217023    0.239266   -2.108120
             1                    2.966423   -0.344295   -1.254206
             6                   -1.866799    0.019966    0.044048
             9                   -1.888808   -0.158027    1.395717
             9                   -2.543899    1.171359   -0.207184
             9                   -2.600865   -0.991960   -0.491180

c

0 1
             6                    0.878684   -1.336513   -0.802238
             6                    1.755168   -1.359712    0.471650
             6                    2.840530   -0.255196    0.522192
             6                    2.448390    1.111897   -0.091500
             6                    0.971820    1.512903    0.135515
            14                   -0.107103    0.278087   -0.807165
             1                    3.127452   -0.110949    1.571848
            1                    1.098456   -1.266489    1.346743
             1                    2.244300   -2.336704    0.575265
             1                    1.501390   -1.402885   -1.704532
             1                    0.209128   -2.204801   -0.825583
             1                    3.116234    1.883145    0.312946
             1                    2.647767    1.093236   -1.172757
             1                    0.728324    1.488623    1.206032
             1                    0.793940    2.539908   -0.202915
             1                   -0.492859    0.750179   -2.165048
             1                    3.743757   -0.609718    0.008813
```

```
             6                   -1.777485    0.006864    0.124444
             9                   -1.581198   -0.430685    1.401713
             9                   -2.509677    1.148475    0.214788
             9                   -2.567024   -0.917593   -0.484378

ts

0 1
             6                    0.850465   -1.503861   -0.386208
             6                    2.047280   -1.254916    0.561456
             6                    3.011099   -0.168066    0.047836
             6                    2.433642    1.282405   -0.053622
             6                    0.917016    1.434621    0.229425
            14                   -0.080053    0.119506   -0.679614
             1                    3.895699   -0.154976    0.695388
             1                    1.679805   -0.987355    1.561305
             1                    2.611888   -2.187732    0.689391
             1                    1.213007   -1.898594   -1.344613
             1                    0.180800   -2.268224    0.026946
             1                    2.978973    1.936229    0.637799
             1                    2.641262    1.677665   -1.055351
             1                    0.720120    1.308291    1.302748
             1                    0.589234    2.449448   -0.022612
             1                   -0.290996    0.431503   -2.120041
             1                    3.373607   -0.483329   -0.940236
             6                   -1.858130    0.017254    0.066962
             9                   -1.831863   -0.246246    1.404057
             9                   -2.553162    1.174996   -0.087468
             9                   -2.601741   -0.966598   -0.506725
```

Converged Path:

```
Min E( 1) =  -824.491659717
    E( 2) =  -824.491619356
    E( 3) =  -824.491506193
    E( 4) =  -824.491368193
    E( 5) =  -824.491252249
TS  E( 6) =  -824.491199817
    E( 7) =  -824.491318217
    E( 8) =  -824.491743232
    E( 9) =  -824.492349422
    E(10) =  -824.492851535
Min E(11) =  -824.493065887
```

*Structure **5e–5d**:*

*B3LYP/6-311+G** STQN(Path) calculation input file*

```
#b3lyp/6-311+G** opt(qst3,path=11)

e

0 1
             6                    -0.096449    1.504419   -0.027492
             6                     1.404218    1.299376    0.293588
             6                     2.028434    0.065869   -0.386645
             6                     1.460008   -1.284073    0.091197
             6                    -0.030188   -1.501628   -0.267862
            14                    -1.070836   -0.061991    0.365548
             1                     1.900449    0.148036   -1.476505
             1                     1.963642    2.195417   -0.006192
             1                     1.538428    1.209391    1.381592
             1                    -0.492195    2.372035    0.513692
             1                    -0.214767    1.725345   -1.097822
             1                     2.058110   -2.097623   -0.340234
             1                     1.591252   -1.358188    1.180809
             1                    -0.138861   -1.554422   -1.360434
             1                    -0.387192   -2.460579    0.126151
             1                    -1.377889   -0.186150    1.817486
             1                     3.110707    0.075149   -0.204133
             6                    -2.789179   -0.029008   -0.515024
             9                    -2.666401    0.109730   -1.864979
             9                    -3.496523   -1.170916   -0.304423
             9                    -3.568563    0.999812   -0.088150

d

0 1
             6                    -0.064951   -1.329527   -0.792851
             6                     1.223804   -1.418120    0.074885
             6                     1.732782   -0.081819    0.676561
             6                     1.485156    1.158780   -0.202938
             6                     0.006556    1.622384   -0.163113
            14                    -1.158953    0.139860   -0.353870
             1                     1.249478    0.086316    1.648658
             1                     1.051303   -2.119686    0.898777
             1                     2.019645   -1.859994   -0.538120
             1                     0.208352   -1.177086   -1.846902
             1                    -0.615399   -2.276650   -0.766799
             1                     2.130684    1.980811    0.131348
             1                     1.781900    0.942779   -1.238816
             1                    -0.197555    2.118551    0.795055
             1                    -0.189209    2.370442   -0.940944
             1                    -2.255326    0.353582   -1.336522
             1                     2.804640   -0.181849    0.886351
```

```
             6                   -2.079948   -0.180652    1.316497
             9                   -1.228799   -0.483483    2.338477
             9                   -2.794042    0.904859    1.719762
             9                   -2.957424   -1.215189    1.226818

ts

0 1
             6                   -0.104409   -1.415058   -0.681834
             6                    1.332143   -1.398285   -0.067603
             6                    1.749480   -0.111523    0.674831
             6                    1.505209    1.178689   -0.130433
             6                    0.019838    1.617549   -0.126942
            14                   -1.135683    0.134440   -0.354840
             1                    1.216102   -0.043084    1.633931
             1                    1.440609   -2.243899    0.621149
             1                    2.055957   -1.571836   -0.874120
             1                   -0.042933   -1.523200   -1.772360
             1                   -0.663490   -2.294348   -0.339924
             1                    2.122028    1.991291    0.273775
             1                    1.845128    1.025212   -1.164647
             1                   -0.219703    2.095347    0.832436
             1                   -0.165436    2.375810   -0.897072
             1                   -2.174250    0.337930   -1.400792
             1                    2.814651   -0.194728    0.925295
             6                   -2.156547   -0.104778    1.269882
             9                   -1.365867   -0.354818    2.352565
             9                   -2.891339    0.998153    1.577250
             9                   -3.028793   -1.144556    1.181764
```

Converged Path:

```
Min E( 1) =  -824.498903158
    E( 2) =  -824.497834472
    E( 3) =  -824.495572944
    E( 4) =  -824.493373989
    E( 5) =  -824.492113821
TS  E( 6) =  -824.491772405
    E( 7) =  -824.491799963
    E( 8) =  -824.491880777
    E( 9) =  -824.491965500
    E(10) =  -824.492020493
Min E(11) =  -824.492035330
```

*Structure **5d–5c**:*

*B3LYP/6-311+G** STQN(Path) calculation input file*

```
#b3lyp/6-311+G** opt(calcfc,qst3,path=11) scf(cdiis,vshift=300) guess(always) nosymm
int=ultrafine

d

0 1
             6                    0.968062   -1.296845   -1.008997
             6                    1.832935   -1.466800    0.273050
             6                    2.165624   -0.164956    1.048344
             6                    2.326501    1.090213    0.169426
             6                    0.964946    1.644681   -0.320051
            14                   -0.120920    0.240895   -0.986820
             1                    1.374641    0.032838    1.784838
             1                    1.323332   -2.152920    0.958785
             1                    2.769845   -1.962921   -0.010550
             1                    1.623513   -1.166556   -1.882233
             1                    0.390589   -2.206229   -1.210085
             1                    2.851351    1.869541    0.736385
             1                    2.967975    0.859391   -0.692626
             1                    0.446551    2.133977    0.515351
             1                    1.110036    2.418193   -1.083904
             1                   -0.731099    0.524665   -2.313842
             1                    3.081278   -0.331797    1.628576
             6                   -1.639731   -0.013470    0.182009
             9                   -1.273980   -0.318255    1.459786
             9                   -2.414388    1.102222    0.259394
             9                   -2.447760   -1.022595   -0.238946

c

0 1
             6                    0.878785   -1.335828   -0.803815
             6                    1.753756   -1.360217    0.471099
             6                    2.839069   -0.255691    0.523948
             6                    2.448404    1.111326   -0.090742
             6                    0.971862    1.513378    0.134564
            14                   -0.107222    0.278596   -0.808061
             1                    3.123687   -0.111314    1.574215
             1                    1.095987   -1.267812    1.345481
             1                    2.242759   -2.337306    0.574384
             1                    1.502579   -1.401036   -1.705447
             1                    0.209393   -2.204187   -0.828948
             1                    3.116316    1.882316    0.314091
             1                    2.648905    1.092048   -1.171776
             1                    0.727309    1.489935    1.204859
             1                    0.794979    2.540285   -0.204701
             1                   -0.494049    0.750654   -2.165650
```

```
             1                   3.743422   -0.610271    0.012599
             6                  -1.776899    0.006829    0.124711
             9                  -1.579402   -0.423582    1.404234
             9                  -2.512751    1.146531    0.209181
             9                  -2.563409   -0.923221   -0.479508

ts

0 1
             6                   0.924796   -1.239901   -1.033784
             6                   1.684817   -1.490764    0.293398
             6                   2.413940   -0.253399    0.913496
             6                   2.400034    1.042284    0.079683
             6                   0.980873    1.623520   -0.123764
            14                  -0.125865    0.321098   -0.940126
             1                   1.965968   -0.026322    1.889955
             1                   0.970450   -1.881686    1.025857
             1                   2.413149   -2.293944    0.127954
             1                   1.635826   -1.103389   -1.860702
             1                   0.325096   -2.119735   -1.295005
             1                   3.030101    1.786565    0.584110
             1                   2.872086    0.863874   -0.896504
             1                   0.558444    1.911634    0.848320
             1                   1.019354    2.538539   -0.726729
             1                  -0.688504    0.732314   -2.255075
             1                   3.457440   -0.519288    1.119809
             6                  -1.672209   -0.004264    0.172598
             9                  -1.322054   -0.368858    1.440622
             9                  -2.461174    1.096635    0.293067
             9                  -2.460195   -0.999865   -0.312576
```

Converged Path:

```
Min E( 1) =  -824.492020241
    E( 2) =  -824.491960092
    E( 3) =  -824.491801405
    E( 4) =  -824.491586936
    E( 5) =  -824.491409067
TS  E( 6) =  -824.491331907
    E( 7) =  -824.491466186
    E( 8) =  -824.491858604
    E( 9) =  -824.492393709
    E(10) =  -824.492865328
Min E(11) =  -824.493060816
```