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Structure, Stability and Spectral Properties of Seleno[n]helicenes (n=1-10)

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Table of contents

1. Cartesian coordinates for the most stable structures of neutral end substituted seleno[n]helicenes, n=1-10 calculated at B3LYP-D /6-311++G(d,p) level in DCM solvent.

1.1 Neutral seleno[1]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.880567
C	1.752094	0.000000	2.563715
C	-0.915931	-1.540187	2.506555
C	-0.668535	-2.873834	2.337469
Br	0.841208	-3.478180	1.305741
Se	-2.471311	-1.369112	3.569653
C	-2.620273	-3.252161	3.671361
Si	-4.039198	-4.058020	4.640966
C	-5.077085	-5.100633	3.469508
C	-1.583996	-3.793446	2.963099
Br	-1.372735	-5.702165	2.818545
C	-0.940778	1.498210	2.523438
C	-3.325217	-5.101069	6.033382
C	-5.080950	-2.661417	5.353116
H	-4.137854	-5.525239	6.636727
H	-2.719834	-5.929055	5.651362
H	-2.695065	-4.494321	6.694153
H	-5.917914	-3.080575	5.925141
H	-4.499770	-2.025990	6.031532
H	-5.501933	-2.025854	4.565322
H	-5.934812	-5.524533	4.007033
H	-5.463193	-4.493688	2.642228
H	-4.501336	-5.928797	3.044472
H	0.475709	0.915683	-0.373555
H	0.548162	-0.855901	-0.406136
H	-1.023294	-0.033205	-0.391947
H	2.272861	0.915794	2.256405
H	1.745538	-0.033463	3.659476
H	2.329673	-0.855780	2.200339
H	-0.446080	2.417069	2.185227
H	-1.972258	1.520250	2.152838
H	-0.970120	1.520397	3.619079

1.2 Neutral seleno[2]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.881050
C	1.750607	0.000000	2.569327
C	-0.941196	-1.519792	2.522307
Se	-2.506035	-1.248181	3.588540
C	-2.650253	-3.108328	3.686756
Se	-3.879436	-4.238953	4.524248
C	-2.862382	-5.703402	3.831184
Si	-3.431806	-7.473177	4.219102
C	-3.844868	-8.372518	2.619441
C	-1.645607	-3.783840	3.002181
C	-0.721995	-2.858735	2.372891
Br	0.802260	-3.426238	1.334235
C	-1.806979	-5.221466	3.112075
Br	-0.603684	-6.487944	2.292119
C	-0.920125	1.519218	2.508000
C	-2.094209	-8.372629	5.188725
C	-4.983857	-7.330156	5.276645
H	-0.408217	2.424623	2.159228
H	-1.950353	1.556607	2.135092
H	-0.950037	1.556583	3.603232
H	0.473285	0.917812	-0.371698
H	0.548147	-0.853914	-0.409392
H	-1.024073	-0.033227	-0.390114
H	2.269706	0.917809	2.264861
H	1.738960	-0.033238	3.665128
H	2.332180	-0.853908	2.208979
H	-5.348849	-8.334349	5.525299
H	-4.789869	-6.805283	6.219355
H	-5.790216	-6.805219	4.751236
H	-2.453316	-9.367230	5.482578
H	-1.179950	-8.502033	4.601678
H	-1.838160	-7.823008	6.102164
H	-4.249770	-9.367116	2.846083
H	-4.601279	-7.822832	2.046985
H	-2.964037	-8.501919	1.983339

1.3 Neutral seleno[3]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.881687
C	1.777235	0.000000	2.506888
C	-0.905027	-1.500201	2.566110
C	-0.809708	1.588289	2.529214
Se	0.299519	2.922174	3.326392
C	-1.244612	3.957449	3.506078
Se	-1.452328	5.771555	3.981032
C	-3.284259	5.455417	3.658853
Se	-4.762088	6.577572	3.871133
C	-5.848004	5.032446	3.590951
Si	-7.732473	5.211130	3.711052
C	-8.356204	4.392842	5.286522
C	-2.101447	2.034957	2.503028
C	-2.412742	3.315416	3.111345
C	-3.604730	4.145044	3.322967
C	-5.041738	3.949036	3.378793
Br	-5.855221	2.202470	3.477314
Br	-3.351963	1.074358	1.391539
C	-8.101986	7.057356	3.777008
C	-8.540901	4.464399	2.185618
H	-0.389122	-2.418472	2.257529
H	-0.926288	-1.477023	3.662015
H	-1.937144	-1.554789	2.207160
H	0.530665	-0.884866	-0.374155
H	-1.015733	-0.015737	-0.406786
H	0.509560	0.889117	-0.389790
H	2.286602	-0.906908	2.158334
H	2.343893	0.860761	2.132462
H	1.824027	0.008400	3.601985
H	-9.186254	7.210252	3.843465
H	-7.647464	7.535750	4.652651
H	-7.746724	7.576414	2.879308
H	-9.436344	4.557029	5.391049
H	-8.175328	3.313623	5.283445
H	-7.863133	4.818593	6.168414
H	-9.624103	4.638655	2.215830
H	-8.150201	4.925935	1.271105
H	-8.373287	3.385188	2.120105

1.4 Neutral seleno[4]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.883182
C	1.772229	0.000000	2.516197
C	-0.949818	-1.491444	2.524306
C	-0.878924	1.584056	2.435976
C	-1.304337	2.002891	3.663091
Br	-0.652090	1.116276	5.251162
Se	-1.230723	2.966463	1.154834
C	-1.920303	3.979020	2.573783
C	-1.981936	3.274231	3.766084
C	-2.528202	4.047833	4.867925
C	-3.019792	3.734266	6.198690
C	-3.574044	2.553092	6.818128
Br	-4.105833	1.044319	5.734480
Se	-2.279294	5.827674	2.764780
C	-2.596177	5.399293	4.583331
Se	-2.989478	6.490441	6.081917
C	-3.172951	4.849658	7.007686
Se	-3.790597	4.432326	8.727729
C	-3.981939	2.624516	8.118353
Si	-4.715577	1.320222	9.279352
C	-6.466433	0.895269	8.735828
C	-3.614050	-0.204312	9.273313
C	-4.753662	2.077811	11.003006
H	-6.916249	0.183453	9.439821
H	-7.097085	1.791796	8.712261
H	-6.481409	0.442983	7.739223
H	-5.175448	1.357369	11.714671
H	-3.748472	2.342099	11.351216
H	-5.376258	2.979876	11.038236
H	-3.999975	-0.949514	9.980561
H	-3.569426	-0.668047	8.282930
H	-2.591777	0.051717	9.575474
H	-0.479827	-2.417350	2.168958
H	-0.969714	-1.519514	3.618252
H	-1.985641	-1.478134	2.165434
H	0.503370	-0.901702	-0.370082
H	-1.018678	0.003961	-0.404705
H	0.533617	0.866948	-0.407732
H	2.302520	-0.888059	2.149092
H	2.313204	0.886333	2.164349
H	1.810423	-0.009428	3.610026

1.5 Neutral seleno[5]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.881167
C	1.787633	0.000000	2.503932
Se	2.350280	-1.316312	3.778712
C	4.025129	-0.474785	3.768095
C	4.121392	0.542289	2.831864
C	5.421600	1.196041	2.812942
C	6.070248	2.175315	1.954740
C	7.143686	2.797087	2.570311
Se	7.886971	4.237022	1.589224
C	6.660069	3.719686	0.245597
Se	6.441742	4.264459	-1.534560
C	5.373531	2.692526	-1.784106
Si	4.664345	2.301177	-3.495060
C	2.811755	2.010803	-3.345467
C	-0.807339	-1.575188	2.524938
C	-0.914127	1.499354	2.557920
C	2.839726	0.822626	2.228939
Br	2.536410	2.486061	1.299606
Se	5.499575	-0.568702	4.949386
C	6.188089	0.862660	3.917125
Se	7.681735	1.989114	4.193240
C	5.911195	2.600320	0.571860
C	5.295001	2.022461	-0.599126
Br	4.638179	0.208560	-0.567100
C	4.994880	3.801644	-4.584466
C	5.529414	0.794144	-4.217690
H	4.597581	3.623155	-5.591315
H	4.512127	4.703572	-4.190505
H	6.068222	4.003196	-4.683488
H	5.162618	0.602214	-5.234178
H	6.612644	0.954007	-4.273630
H	5.348856	-0.102430	-3.616478
H	2.378610	1.818576	-4.335364
H	2.588615	1.152502	-2.704313
H	2.311916	2.889598	-2.921697
H	-1.029837	-0.037083	-0.377519
H	0.477698	0.898202	-0.403221
H	0.535657	-0.873179	-0.390295
H	-1.966545	1.468837	2.247906
H	-0.884712	1.513900	3.653819

H	-0.479797	2.435698	2.193888
H	-1.849676	-1.622353	2.186179
H	-0.296314	-2.472701	2.157441
H	-0.814014	-1.609531	3.620962

1.6 Neutral seleno[6]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.884148
C	1.774082	0.000000	2.513638
C	-0.944610	1.497957	2.512573
C	-0.862526	-1.592125	2.438883
C	-1.197123	-2.066483	3.673382
Br	-0.618301	-1.107193	5.239980
Se	-1.286180	-2.922036	1.129720
C	-1.845200	-4.005080	2.550051
C	-1.810326	-3.370753	3.781780
C	-2.263668	-4.213693	4.884293
C	-2.521724	-4.022984	6.310031
C	-2.808831	-2.889967	7.187258
C	-3.329773	-1.537413	7.011770
C	-4.004757	-0.828647	5.948314
Br	-4.584368	-1.743742	4.355780
Se	-2.244970	-5.848082	2.636633
C	-2.377717	-5.539561	4.498393
Se	-2.491540	-6.769529	5.925947
C	-2.484898	-5.222145	7.008050
Se	-2.436161	-5.044141	8.887236
C	-2.644561	-3.202803	8.527060
Se	-2.812964	-1.743218	9.718791
C	-3.299045	-0.778142	8.170781
Se	-3.945104	0.964027	7.946525
C	-4.393894	0.462390	6.155151
Si	-5.343005	1.689384	5.068769
C	-5.393657	3.326568	5.999944
C	-4.451394	1.924984	3.431515
C	-7.097658	1.060826	4.804709
H	-5.917970	3.235979	6.958610
H	-4.386804	3.714070	6.194755
H	-5.927743	4.074044	5.400275
H	-5.021137	2.609863	2.790420
H	-3.458350	2.356650	3.590119
H	-4.328252	0.979670	2.894988
H	1.814969	0.014663	3.607286

H	2.312622	-0.889121	2.165117
H	2.304888	0.885439	2.140956
H	-1.951897	1.527420	2.085803
H	-1.038341	1.492660	3.602450
H	-0.424164	2.418620	2.218996
H	0.483066	0.913875	-0.367492
H	0.553159	-0.853666	-0.409166
H	-1.018084	-0.024392	-0.405920
H	-7.109750	0.115872	4.252560
H	-7.604114	0.900725	5.763823
H	-7.678280	1.796592	4.233591

1.7 Neutral seleno[7]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.878697
C	1.776712	0.000000	2.506642
C	-0.793100	-1.602748	2.492641
Se	0.158453	-2.686159	3.745862
C	-1.311900	-3.837635	3.721239
C	-2.299845	-3.467684	2.820544
C	-1.999882	-2.185490	2.227336
Br	-3.376368	-1.140506	1.372511
Se	-1.768609	-5.299126	4.821464
C	-3.384629	-5.290826	3.841260
Se	-4.954166	-6.307731	4.086356
C	-5.545555	-5.406979	2.537787
Se	-7.236107	-5.414773	1.699487
C	-6.386694	-4.324189	0.415000
Se	-7.093303	-3.473262	-1.113328
C	-5.292436	-3.032707	-1.460315
Se	-4.543250	-2.001648	-2.856030
C	-2.894658	-2.552752	-2.125651
Se	-1.139725	-2.309531	-2.716835
C	-0.619939	-3.579649	-1.387768
Si	1.204699	-4.050518	-1.233759
C	1.475816	-5.822054	-1.807598
C	-3.428955	-4.392305	2.788109
C	-4.596964	-4.592876	1.934629
C	-5.025349	-4.139361	0.612414
C	-4.379003	-3.555332	-0.559785
C	-3.006588	-3.398194	-1.031650
C	-1.732251	-3.999588	-0.714963
Br	-1.627595	-5.594546	0.363270

C	-0.918249	1.491721	2.566244
C	1.746853	-3.815955	0.549653
C	2.164611	-2.867335	-2.342660
H	1.825751	-0.005571	3.602045
H	2.332227	-0.868735	2.134334
H	2.293378	0.902344	2.156958
H	0.450849	0.925856	-0.379849
H	0.580495	-0.844087	-0.385201
H	-1.012680	-0.077656	-0.404958
H	0.950858	-6.538018	-1.167507
H	1.118908	-5.959495	-2.835132
H	2.545964	-6.064831	-1.785347
H	1.631447	-2.770735	0.853027
H	1.158167	-4.430646	1.236054
H	2.803468	-4.089996	0.664651
H	3.238099	-3.082105	-2.272357
H	1.876064	-2.965424	-3.395971
H	2.011956	-1.824386	-2.041222
H	-1.948506	1.535238	2.199395
H	-0.948602	1.461686	3.661814
H	-0.409736	2.417088	2.266639

1.8 Neutral seleno[8]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.884895
C	1.772938	0.000000	2.520432
C	-0.832842	-1.607632	2.433478
C	-1.181517	-2.103027	3.655596
Br	-0.695456	-1.130362	5.246828
C	-1.670818	-3.460842	3.748424
C	-2.089886	-4.338696	4.835915
C	-2.603687	-4.166973	6.194326
C	-3.162296	-3.068640	6.987431
C	-3.635065	-1.705302	6.732091
C	-3.941308	-0.892769	5.555330
C	-4.154871	-1.136106	4.132634
C	-4.571365	-2.269091	3.336034
Br	-5.257131	-3.858241	4.183782
C	-1.548210	-4.112872	2.530925
Se	-1.678959	-5.987928	2.638665
C	-1.997368	-5.672594	4.470546

Se	-2.279153	-6.906998	5.863164
C	-2.605610	-5.365070	6.895848
Se	-2.997946	-5.227611	8.732281
C	-3.272233	-3.408177	8.330215
Se	-3.674940	-1.985216	9.496506
C	-3.786773	-0.981752	7.907209
Se	-4.010777	0.876404	7.688972
C	-4.028306	0.457913	5.854008
Se	-4.074709	1.613008	4.363972
C	-4.114868	0.017730	3.364961
Se	-4.364055	-0.284497	1.538931
C	-4.709478	-2.114780	1.987865
Si	-5.385797	-3.239241	0.625066
C	-5.097688	-2.349013	-1.011183
Se	-1.034609	-2.994022	1.126572
C	-0.918688	1.517192	2.499796
C	-4.513833	-4.901122	0.582726
C	-7.233697	-3.471026	0.905718
H	-5.630128	-1.391805	-1.059275
H	-4.031835	-2.157962	-1.182480
H	-5.462492	-2.971983	-1.837194
H	-4.979777	-5.532082	-0.185452
H	-3.455752	-4.781711	0.329948
H	-4.578670	-5.424911	1.539427
H	1.805045	0.004982	3.614939
H	2.314413	-0.886244	2.169289
H	2.305779	0.889287	2.160152
H	-1.920264	1.572427	2.062205
H	-1.021174	1.524045	3.587588
H	-0.365444	2.417572	2.202231
H	0.462499	0.924570	-0.367061
H	0.570055	-0.840818	-0.412450
H	-1.018961	-0.046063	-0.401851
H	-7.432476	-3.991106	1.848588
H	-7.749052	-2.503878	0.936653
H	-7.670384	-4.063420	0.091515

1.9 Neutral seleno[9]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.890568
C	1.784573	0.000000	2.491455
C	-0.919319	-1.529285	2.500536

C	-0.917281	1.563547	2.451035
Se	-1.894728	2.550820	1.135850
C	-2.546349	3.594649	2.540372
Se	-4.031331	4.752390	2.622906
C	-3.693727	4.755382	4.479907
Se	-4.761373	5.395936	5.893436
C	-3.379944	4.731036	6.986779
Se	-3.237813	4.698282	8.864372
C	-1.497646	4.059204	8.527863
Se	-0.156782	3.516199	9.734664
C	0.915563	3.408908	8.189443
Se	2.668091	2.749771	7.979622
C	2.452477	3.297513	6.190733
Se	3.582376	3.040737	4.706409
C	2.286886	4.051028	3.784857
Se	2.267977	4.632297	1.989245
C	0.829329	5.714812	2.546740
Se	-0.044077	7.118483	1.678550
C	-0.725910	7.626204	3.392378
C	-0.280684	6.734604	4.326298
Br	-0.474114	7.159892	6.190944
C	-1.151449	2.112815	3.679395
C	-1.991620	3.288718	3.774696
C	-2.551029	4.077606	4.874494
C	-2.279311	4.235788	6.304378
C	-1.133377	4.029263	7.191227
C	0.306858	3.835513	7.020001
C	1.258225	3.944692	5.913070
C	1.259929	4.541023	4.575987
C	0.526887	5.611594	3.896748
Br	-0.622488	1.143211	5.252682
Si	-1.685212	9.258202	3.520980
C	-0.621979	10.554089	4.384769
C	-2.041794	9.836898	1.756839
C	-3.323572	9.021020	4.418359
H	-1.128618	10.038067	1.188945
H	-2.639365	9.111520	1.197061
H	-2.611453	10.771198	1.791013
H	-3.863068	9.973074	4.463499
H	-3.955498	8.301518	3.890986
H	-3.185696	8.661086	5.439340
H	-0.943533	-1.578910	3.591110
H	-1.952139	-1.534547	2.140729
H	-0.429850	-2.436477	2.130719
H	2.326849	0.864985	2.100465

H	1.852632	0.025713	3.580341
H	2.294214	-0.903559	2.140240
H	0.537978	-0.882314	-0.361524
H	-1.009464	-0.045153	-0.419296
H	0.502435	0.879547	-0.413001
H	-0.390696	10.268111	5.412935
H	0.323953	10.700290	3.855581
H	-1.145242	11.515810	4.409970

1.10 Neutral seleno[10]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.882495
C	1.789379	0.000000	2.481526
C	-0.828998	-1.561329	2.579715
C	-2.051190	-2.138744	2.381750
Br	-3.369470	-1.198099	1.336725
Se	0.076768	-2.504370	3.979159
C	-1.446623	-3.575126	4.115262
Se	-2.001628	-4.742369	5.485321
C	-3.613830	-4.817744	4.507512
Se	-5.275506	-5.550066	5.007315
C	-5.842840	-4.914744	3.326954
Se	-7.568999	-4.880304	2.572440
C	-6.680873	-4.194340	1.059188
Se	-7.386577	-3.643859	-0.599275
C	-5.574124	-3.484848	-1.092444
Se	-4.815314	-2.834771	-2.690913
C	-3.189341	-3.371064	-1.903413
Se	-1.421863	-3.094910	-2.494191
C	-0.961594	-4.079505	-0.955083
Se	0.737279	-4.500398	-0.258085
C	-0.237452	-5.552906	0.962327
Se	0.396379	-6.675109	2.340702
C	-1.389379	-7.268745	2.419629
Se	-2.152035	-8.694125	3.353659
C	-3.673868	-8.505788	2.206176
Si	-5.046496	-9.813837	2.332702
C	-4.938570	-10.993903	0.866094
C	-2.412415	-3.311050	3.153928
C	-3.609393	-4.145432	3.294434
C	-4.842685	-4.368077	2.534254
C	-5.299411	-4.140241	1.160815

C	-4.664304	-3.908945	-0.138021
C	-3.308470	-4.013578	-0.680782
C	-2.036160	-4.591560	-0.240341
C	-1.606649	-5.589163	0.743905
C	-2.233528	-6.689259	1.482482
C	-3.453475	-7.461378	1.353627
Br	-4.597012	-7.254532	-0.183998
C	-0.867305	1.534382	2.552270
C	-6.750571	-9.019599	2.428254
C	-4.749128	-10.786969	3.921816
H	1.867513	0.041161	3.572643
H	2.340875	-0.878353	2.131586
H	2.298833	0.886217	2.086644
H	0.538834	0.883364	-0.362014
H	0.506862	-0.886156	-0.393022
H	-1.008124	0.027321	-0.418867
H	-5.129930	-10.488779	-0.084270
H	-3.949409	-11.459328	0.807597
H	-5.679798	-11.793794	0.976278
H	-6.819256	-8.338080	3.281170
H	-7.002638	-8.459067	1.525602
H	-7.507462	-9.801368	2.561215
H	-5.532806	-11.545429	4.028783
H	-3.788652	-11.312156	3.919759
H	-4.788104	-10.147846	4.809574
H	-1.904565	1.602163	2.213939
H	-0.868517	1.539270	3.647010
H	-0.344082	2.435871	2.213244

2 Cartesian coordinates for the most stable structures of radical cations of end substituted seleno[n]helicenes, n=1-10 calculated at B3LYP-D/6-311++G(d,p) level in DCM solvent.

2.1 Seleno[1]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.867536
C	1.749951	0.000000	2.518545
C	-0.951402	-1.529199	2.515045
C	-0.728175	-2.905830	2.354750
Br	0.722770	-3.596405	1.369937
Se	-2.472250	-1.298126	3.548672
C	-2.727293	-3.167229	3.712052
Si	-4.193512	-3.855800	4.724104
C	-5.316896	-4.879464	3.639949
C	-1.690997	-3.810973	3.002572
Br	-1.512960	-5.695395	2.875754
C	-0.902123	1.504154	2.497233
C	-3.555756	-4.877177	6.151058
C	-5.131989	-2.383830	5.376252
H	-4.426665	-5.220886	6.724387
H	-3.000593	-5.760247	5.826311
H	-2.917287	-4.292434	6.822680
H	-5.971262	-2.796641	5.959317
H	-4.551420	-1.749973	6.055288
H	-5.565554	-1.751703	4.593656
H	-6.149303	-5.221282	4.269067
H	-5.736315	-4.299191	2.810744
H	-4.824762	-5.763810	3.229465
H	0.518912	0.910410	-0.327070
H	0.529341	-0.855308	-0.426506
H	-1.015159	0.022135	-0.411857
H	2.233672	0.911042	2.142727
H	1.786153	0.024962	3.613264
H	2.335831	-0.854097	2.171416
H	-0.342817	2.372519	2.112910
H	-1.928979	1.594677	2.126846
H	-0.915441	1.588830	3.589337

2.2 Seleno[2]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.876291
C	1.731000	0.000000	2.600242
C	-0.916624	-1.572884	2.486526
Se	-2.467409	-1.382738	3.518823
C	-2.576919	-3.238396	3.591764
Se	-3.776650	-4.414679	4.390380
C	-2.754074	-5.828134	3.709790
Si	-3.296503	-7.634210	4.070918
C	-3.663388	-8.484278	2.438972
C	-1.553408	-3.876201	2.910493
C	-0.646667	-2.923792	2.306907
Br	0.876590	-3.421592	1.293015
C	-1.679312	-5.315192	2.994335
Br	-0.463264	-6.524391	2.184919
C	-0.987972	1.455503	2.534001
C	-1.932592	-8.484153	5.039324
C	-4.856040	-7.502194	5.108983
H	-0.507526	2.388073	2.214146
H	-2.014314	1.464440	2.148859
H	-1.028627	1.464452	3.629473
H	0.419528	0.948409	-0.358667
H	0.601085	-0.812236	-0.419042
H	-1.019250	-0.086983	-0.393290
H	2.223784	0.948389	2.351545
H	1.700566	-0.086933	3.692318
H	2.349493	-0.812261	2.207399
H	-5.213949	-8.511129	5.347257
H	-4.676613	-6.983370	6.057888
H	-5.662195	-6.983430	4.577205
H	-2.278661	-9.478344	5.349075
H	-1.019904	-8.615238	4.450732
H	-1.681346	-7.918603	5.943836
H	-4.082666	-9.478475	2.638733
H	-4.400857	-7.918800	1.858037
H	-2.768125	-8.615349	1.824194

2.3 Seleno[3]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.877879
C	1.734389	0.000000	2.595755
C	-0.903557	-1.571928	2.497667
C	-0.541944	-2.916268	2.438258
Br	0.886011	-3.410878	1.276144
C	-0.986711	1.458624	2.531429
C	-1.389294	-3.868578	3.079655
C	-2.562357	-3.260796	3.530282
Se	-3.920126	-4.455049	3.980196
C	-2.685552	-5.796099	3.593401
C	-1.415143	-5.326684	3.255392
C	-0.455633	-6.381312	3.313626
Br	1.423399	-6.073983	3.408412
C	-0.919238	-7.678919	3.520583
Si	0.009616	-9.354608	3.548997
C	-1.315885	-10.682302	3.641678
Se	-2.770004	-7.654567	3.823205
C	0.989279	-9.508282	1.955229
C	1.104171	-9.416593	5.073643
Se	-2.574349	-1.396875	3.331555
H	2.235459	0.940923	2.335887
H	1.706749	-0.076226	3.688717
H	2.342900	-0.822865	2.209333
H	0.397319	0.957103	-0.360856
H	0.619356	-0.800996	-0.413965
H	-1.016868	-0.112288	-0.393183
H	-0.507910	2.390452	2.206820
H	-2.013395	1.466289	2.147171
H	-1.025772	1.469518	3.626581
H	-0.836015	-11.668414	3.656922
H	-1.920309	-10.597587	4.552331
H	-1.986817	-10.653011	2.775657
H	1.536902	-10.420696	5.166620
H	1.926631	-8.697226	5.022311
H	0.525125	-9.213942	5.981860
H	1.448404	-10.503592	1.905187
H	0.337745	-9.393539	1.081457
H	1.789213	-8.765192	1.887139

2.4 Seleno[4]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.879685
C	1.760241	0.000000	2.535677
C	-0.996032	-1.448904	2.538660
C	-0.862264	1.613216	2.415502
C	-1.288287	2.049893	3.631773
Br	-0.688216	1.182103	5.235489
Se	-1.188917	2.994822	1.114663
C	-1.854089	4.030557	2.488356
C	-1.940328	3.344214	3.699368
C	-2.534027	4.119357	4.740616
C	-3.086730	3.849750	6.028776
C	-3.641961	2.677774	6.679262
Br	-4.147745	1.142772	5.643405
Se	-2.262439	5.890469	2.612163
C	-2.588827	5.515326	4.410701
Se	-2.973659	6.629487	5.857266
C	-3.244941	4.996516	6.806560
Se	-3.855397	4.637903	8.509784
C	-4.055731	2.800542	7.969695
Si	-4.805143	1.537968	9.185158
C	-6.548754	1.114090	8.629353
C	-3.692902	0.025715	9.225982
C	-4.838121	2.378200	10.866272
H	-7.016686	0.440884	9.358661
H	-7.167964	2.015667	8.556559
H	-6.556566	0.614665	7.655491
H	-5.253646	1.690808	11.613097
H	-3.832373	2.661474	11.197773
H	-5.465141	3.277851	10.861952
H	-4.065024	-0.686154	9.973451
H	-3.660567	-0.486725	8.259612
H	-2.668419	0.300998	9.502011
H	-0.559046	-2.389994	2.181822
H	-1.007183	-1.476156	3.632572
H	-2.033125	-1.402930	2.186714
H	0.478426	-0.915772	-0.367951
H	-1.018031	0.029701	-0.405461
H	0.558349	0.850455	-0.409287
H	2.289576	-0.891394	2.176125
H	2.309450	0.882214	2.186924
H	1.788009	-0.009305	3.629768

2.5 Seleno[5]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.878788
C	1.805857	0.000000	2.479062
Se	2.394669	-1.322124	3.720602
C	4.064310	-0.504727	3.675378
C	4.139288	0.531271	2.763349
C	5.437259	1.175703	2.735670
C	6.100488	2.073830	1.863991
C	7.229461	2.682211	2.469477
Se	7.911131	4.128924	1.524877
C	6.647834	3.645675	0.184229
Se	6.409907	4.212206	-1.570856
C	5.320480	2.669396	-1.833581
Si	4.551650	2.330808	-3.541124
C	2.701796	2.087498	-3.320481
C	-0.784523	-1.575616	2.540763
C	-0.886453	1.504219	2.573982
C	2.853244	0.829905	2.185428
Br	2.547174	2.494458	1.278992
Se	5.578501	-0.622727	4.824327
C	6.232450	0.820357	3.854904
Se	7.772744	1.888317	4.096016
C	5.906875	2.522106	0.499313
C	5.254390	1.968541	-0.660381
Br	4.572165	0.174054	-0.639703
C	4.898515	3.848911	-4.595306
C	5.366208	0.817173	-4.300846
H	4.471794	3.707637	-5.595832
H	4.450535	4.753272	-4.167303
H	5.974496	4.022167	-4.717131
H	4.974446	0.655551	-5.313096
H	6.451534	0.951532	-4.376716
H	5.173963	-0.087365	-3.715648
H	2.223192	1.950359	-4.298269
H	2.477752	1.208561	-2.708333
H	2.246802	2.961318	-2.840072
H	-1.029652	-0.061183	-0.374181
H	0.453732	0.909115	-0.406310
H	0.554421	-0.860768	-0.391243
H	-1.945033	1.475117	2.286215
H	-0.834892	1.519412	3.668904

H	-0.459830	2.439554	2.198821
H	-1.832066	-1.628214	2.219843
H	-0.276606	-2.472114	2.166530
H	-0.773502	-1.605880	3.636920

2.6 Seleno[6]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.881850
C	1.764577	0.000000	2.522221
C	-0.873893	1.597467	2.432209
Se	-1.739002	2.677494	1.122437
C	-2.330216	3.749370	2.532421
Se	-3.661402	5.088017	2.627057
C	-3.371647	5.020689	4.464094
Se	-4.321009	5.855845	5.886780
C	-3.058867	5.004894	6.966874
Se	-2.945422	4.866397	8.825401
C	-1.251068	4.079600	8.460881
Se	0.034536	3.409469	9.626188
C	1.120898	3.261608	8.085691
Se	2.934087	2.869887	7.873108
C	2.766035	3.514865	6.088253
Si	4.322880	3.636666	5.002435
C	4.026158	2.756060	3.371508
C	0.512515	3.711310	6.926677
C	1.470222	3.894989	5.868212
Br	1.015028	4.871699	4.278013
C	-0.897695	4.037238	7.109386
C	-2.001102	4.355158	6.251886
C	-2.318260	4.194817	4.862544
C	-1.835542	3.362669	3.766019
C	-1.089246	2.135839	3.671472
Br	-0.613955	1.142147	5.245491
C	-0.974652	-1.474255	2.524382
C	4.737097	5.453151	4.747142
C	5.708646	2.786976	5.949973
H	5.911431	3.279342	6.908458
H	5.480586	1.732688	6.145266
H	6.632010	2.823171	5.358899
H	4.912950	2.853224	2.732372
H	3.842354	1.689910	3.535158
H	3.170878	3.170566	2.829942

H	-0.976881	-1.516750	3.617966
H	-2.015282	-1.435272	2.181957
H	-0.529852	-2.404696	2.149198
H	2.331724	0.830775	2.091545
H	1.806316	0.087547	3.611827
H	2.262880	-0.935054	2.236565
H	0.506298	-0.902033	-0.365085
H	-1.016602	-0.003297	-0.410716
H	0.533054	0.867410	-0.406432
H	3.953289	5.975588	4.189885
H	4.870354	5.963008	5.708390
H	5.673757	5.545005	4.182765

2.7 Seleno[7]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.877350
C	1.767459	0.000000	2.526423
C	-0.792353	-1.619688	2.470089
Se	0.172461	-2.730125	3.678142
C	-1.291789	-3.883786	3.634951
C	-2.290139	-3.488132	2.757238
C	-2.003755	-2.195213	2.193074
Br	-3.378767	-1.138749	1.359975
Se	-1.741170	-5.379613	4.691060
C	-3.348782	-5.352365	3.750384
Se	-4.910008	-6.418880	3.978640
C	-5.533943	-5.474017	2.501803
Se	-7.225164	-5.465552	1.702738
C	-6.371176	-4.368944	0.407425
Se	-7.087525	-3.456517	-1.037428
C	-5.291635	-3.005929	-1.428673
Se	-4.570196	-1.955140	-2.813909
C	-2.912811	-2.530720	-2.139514
Se	-1.166365	-2.259444	-2.739345
C	-0.624936	-3.561159	-1.448676
Si	1.214122	-4.002150	-1.308564
C	1.505569	-5.760608	-1.906571
C	-3.414696	-4.415283	2.724568
C	-4.564890	-4.619426	1.881978

C	-4.987537	-4.194299	0.583855
C	-4.360252	-3.567793	-0.576448
C	-3.002620	-3.406645	-1.062164
C	-1.724680	-4.008332	-0.772613
Br	-1.601588	-5.619002	0.279455
C	-0.936517	1.468027	2.585957
C	1.736758	-3.773035	0.480910
C	2.139592	-2.787370	-2.410739
H	1.803236	-0.016121	3.621935
H	2.330690	-0.862228	2.149984
H	2.282870	0.909500	2.194203
H	0.445953	0.927163	-0.381783
H	0.587025	-0.841604	-0.381810
H	-1.011863	-0.084045	-0.405802
H	1.018267	-6.500203	-1.264128
H	1.124333	-5.891239	-2.926184
H	2.581858	-5.974716	-1.918569
H	1.573683	-2.736973	0.794121
H	1.168853	-4.421481	1.153518
H	2.802976	-4.002703	0.602107
H	3.218245	-2.977405	-2.351898
H	1.845635	-2.882520	-3.462557
H	1.962615	-1.752222	-2.095380
H	-1.957352	1.533686	2.198158
H	-0.990968	1.401157	3.678962
H	-0.413180	2.398045	2.330159

2.8 Seleno[8]helicene radical cation

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.883001
C	1.765979	0.000000	2.533630
C	-0.818799	-1.623032	2.426116
C	-1.176402	-2.120518	3.642760
Br	-0.746742	-1.142536	5.245890
C	-1.633004	-3.490914	3.727629
C	-2.076314	-4.368573	4.791853
C	-2.613016	-4.206613	6.144096
C	-3.232292	-3.149937	6.901273
C	-3.740245	-1.828059	6.641070
C	-3.999433	-1.005009	5.458588
C	-4.170681	-1.234690	4.038253
C	-4.527580	-2.367292	3.211530
Br	-5.221052	-3.973603	4.017719

C	-1.471213	-4.147642	2.510652
Se	-1.609065	-6.016846	2.608736
C	-1.986082	-5.703212	4.424708
Se	-2.300366	-6.927297	5.815826
C	-2.634044	-5.418250	6.842412
Se	-3.115221	-5.309176	8.672089
C	-3.383562	-3.509840	8.281508
Se	-3.820544	-2.111560	9.428878
C	-3.925559	-1.107204	7.825347
Se	-4.123354	0.725151	7.611899
C	-4.083840	0.343625	5.771927
Se	-4.100730	1.514678	4.300024
C	-4.116817	-0.064403	3.285764
Se	-4.263858	-0.353218	1.451249
C	-4.604301	-2.195630	1.862184
Si	-5.209047	-3.308642	0.449696
C	-4.827301	-2.399280	-1.154368
Se	-0.970834	-3.016971	1.117231
C	-0.936019	1.504301	2.501696
C	-4.339738	-4.971786	0.440033
C	-7.067736	-3.529470	0.645948
H	-5.332661	-1.428035	-1.210553
H	-3.750334	-2.232444	-1.273104
H	-5.168570	-2.999132	-2.006925
H	-4.773333	-5.592983	-0.354482
H	-3.271232	-4.854259	0.234645
H	-4.451636	-5.505048	1.386968
H	1.790043	0.003895	3.628476
H	2.311712	-0.884565	2.185129
H	2.300017	0.890626	2.179050
H	-1.932974	1.557224	2.053388
H	-1.046736	1.507196	3.588578
H	-0.383843	2.408048	2.212750
H	0.474828	0.917981	-0.367408
H	0.556875	-0.848514	-0.414455
H	-1.020172	-0.031537	-0.400054
H	-7.312995	-4.060343	1.571856
H	-7.577463	-2.559148	0.665613
H	-7.470967	-4.108452	-0.194482

2.9 Seleno[9]helicene radical cation

C	0.000000	0.000000	0.000000

Si	0.000000	0.000000	1.885763
C	1.776265	0.000000	2.507593
C	-0.959586	-1.486491	2.523642
C	-0.895095	1.599404	2.434278
Se	-1.855119	2.577597	1.101217
C	-2.521127	3.641766	2.471734
Se	-3.991263	4.828564	2.515334
C	-3.684550	4.848802	4.369730
Se	-4.747274	5.507872	5.762933
C	-3.374338	4.862407	6.877201
Se	-3.232813	4.836109	8.751743
C	-1.515151	4.171012	8.452740
Se	-0.176315	3.638445	9.667192
C	0.894273	3.526256	8.120499
Se	2.617754	2.852078	7.881291
C	2.403206	3.383753	6.090784
Se	3.522902	3.135192	4.598244
C	2.236306	4.145006	3.687355
Se	2.189025	4.719884	1.898347
C	0.771531	5.824118	2.484068
Se	-0.109767	7.225497	1.639206
C	-0.773366	7.739234	3.357128
C	-0.323777	6.844813	4.286108
Br	-0.482739	7.266379	6.150302
C	-1.135950	2.166937	3.652891
C	-1.980229	3.347516	3.718318
C	-2.536509	4.157841	4.788476
C	-2.278331	4.342206	6.206692
C	-1.142145	4.129995	7.102135
C	0.275143	3.952974	6.937475
C	1.215960	4.046878	5.822209
C	1.207797	4.648532	4.499360
C	0.483486	5.722070	3.840417
Br	-0.641081	1.219246	5.245121
Si	-1.709573	9.402893	3.483258
C	-0.604944	10.662146	4.338492
C	-2.064529	9.958829	1.716611
C	-3.336313	9.168612	4.400114
H	-1.153444	10.152258	1.142749
H	-2.673284	9.237808	1.163142
H	-2.625333	10.898395	1.743694
H	-3.867636	10.124381	4.451617
H	-3.983402	8.457837	3.879100
H	-3.188949	8.812957	5.421446
H	-0.981979	-1.525995	3.614553

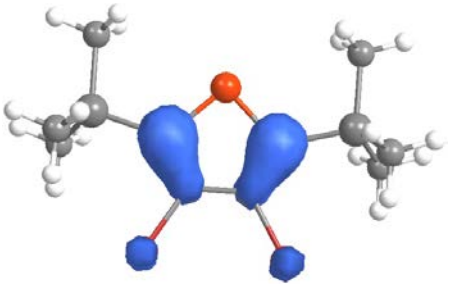
H	-1.992444	-1.473845	2.164921
H	-0.494211	-2.409966	2.164228
H	2.333869	0.850987	2.107246
H	1.834019	0.034376	3.597001
H	2.280148	-0.912856	2.174057
H	0.528704	-0.889334	-0.357178
H	-1.007986	-0.041652	-0.423127
H	0.514113	0.869256	-0.420550
H	-0.376424	10.378857	5.367895
H	0.341107	10.785520	3.804257
H	-1.103072	11.636769	4.361711

2.10 Seleno[10]helicene radical cation

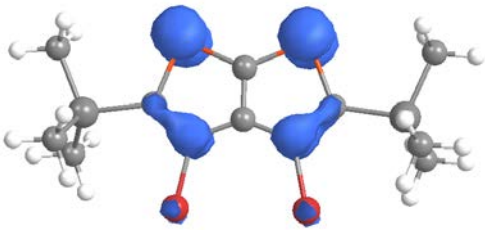
C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.882295
C	1.785793	0.000000	2.486475
C	-0.827650	-1.571101	2.572254
C	-2.048092	-2.151906	2.367966
Br	-3.366370	-1.212161	1.321597
Se	0.074449	-2.513957	3.970250
C	-1.435246	-3.598116	4.092803
Se	-1.975746	-4.793857	5.448419
C	-3.592625	-4.855984	4.494386
Se	-5.236053	-5.623757	4.980020
C	-5.805018	-4.993096	3.300179
Se	-7.522159	-4.925639	2.548043
C	-6.669355	-4.180963	1.066882
Se	-7.381900	-3.637939	-0.601174
C	-5.589139	-3.477951	-1.096036
Se	-4.819052	-2.818348	-2.663327
C	-3.199138	-3.414867	-1.885491
Se	-1.436105	-3.114911	-2.412164
C	-0.981759	-4.108307	-0.887183
Se	0.706121	-4.580251	-0.200426
C	-0.288064	-5.665139	0.966099
Se	0.307746	-6.808216	2.332374
C	-1.485981	-7.391704	2.373844
Se	-2.267387	-8.831595	3.260252
C	-3.784729	-8.592554	2.121088

Si	-5.179842	-9.886395	2.216114
C	-5.082909	-11.025114	0.718288
C	-2.404223	-3.327071	3.137450
C	-3.594404	-4.166342	3.278002
C	-4.809967	-4.406087	2.522939
C	-5.282297	-4.133185	1.163599
C	-4.660726	-3.931515	-0.122373
C	-3.333158	-4.074809	-0.668038
C	-2.068252	-4.650687	-0.205701
C	-1.667054	-5.680301	0.734587
C	-2.315986	-6.783966	1.442725
C	-3.548746	-7.530852	1.293035
Br	-4.689255	-7.269447	-0.238882
C	-0.881648	1.522028	2.557333
C	-6.868068	-9.061549	2.328164
C	-4.896253	-10.897387	3.781857
H	1.859778	0.033781	3.578090
H	2.341967	-0.873498	2.131962
H	2.292925	0.891209	2.100291
H	0.535090	0.887166	-0.357993
H	0.513733	-0.881340	-0.395174
H	-1.007726	0.026126	-0.420133
H	-5.273277	-10.495367	-0.218724
H	-4.097720	-11.496637	0.645545
H	-5.829660	-11.822051	0.809993
H	-6.928500	-8.401661	3.198650
H	-7.110064	-8.477127	1.437886
H	-7.637281	-9.834337	2.440676
H	-5.688426	-11.649322	3.869202
H	-3.941999	-11.433538	3.768440
H	-4.929623	-10.279286	4.684546
H	-1.915872	1.590604	2.210139
H	-0.892436	1.517450	3.651902
H	-0.358309	2.428132	2.231372

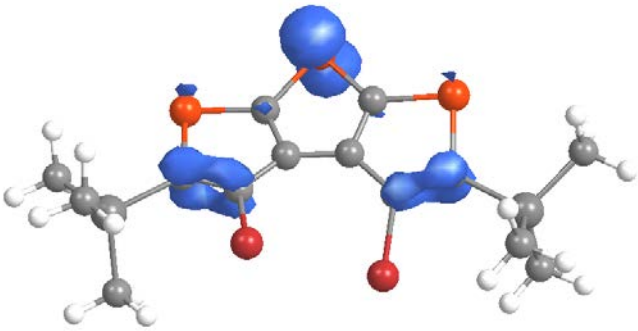
3. Spin density plot with contour cutoff = 0.004 a.u. for the most stable structures of end substituted seleno[n]helicenes radical cation, $[n]SH^{+\ddot{I}}$, n=1-10 (S1a-S1j) at B3LYP-D/6-311++G(d,p) level of theory in DCM solvent following ROHF formalism.



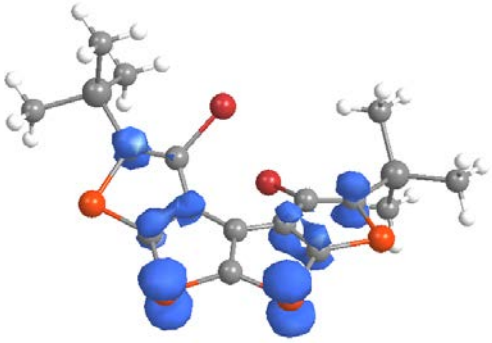
$[1]SH^{+\ddot{I}}$
S1a



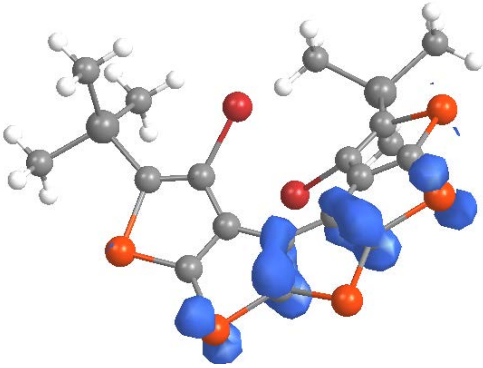
$[2]SH^{+\ddot{I}}$
S1b



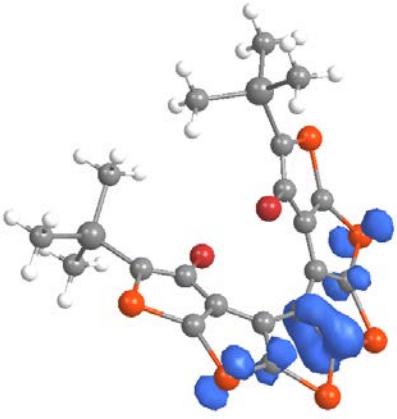
$[3]SH^{+\ddot{I}}$
S1c



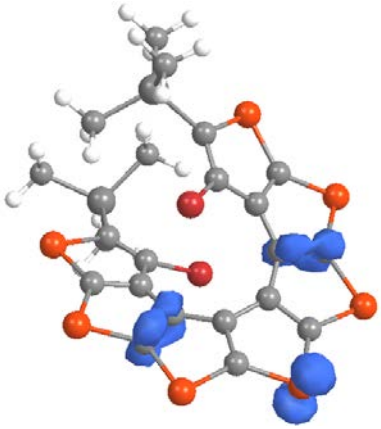
$[4]SH^{+\ddot{I}}$
S1d



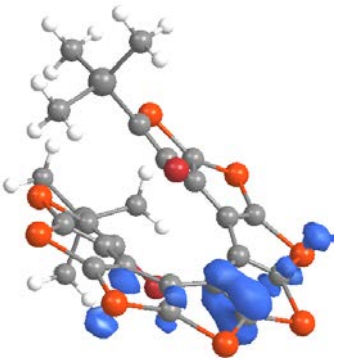
$[5]SH^{+\ddot{I}}$
S1e



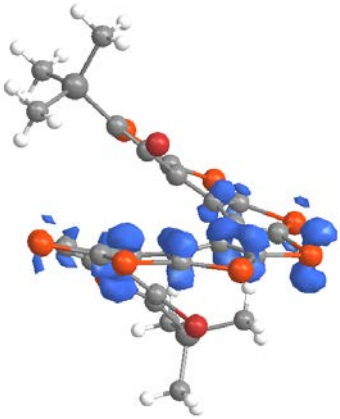
$[6]SH^{+\ddot{I}}$
S1f



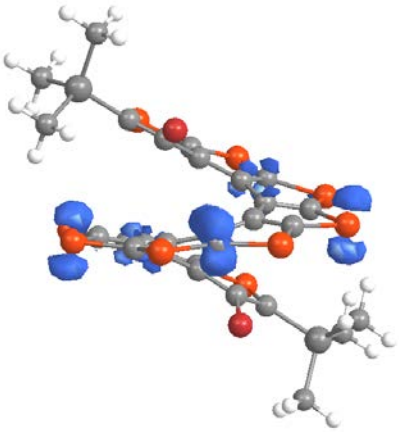
[7]SH$^{+\ddot{I}}$
S1g



[8]SH$^{+\ddot{I}}$
S1h



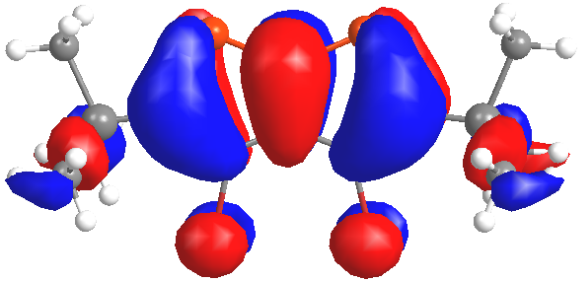
[9]SH$^{+\ddot{I}}$
S1i



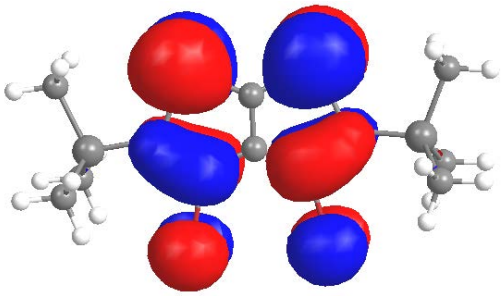
[10]SH$^{+\ddot{I}}$
S1j

Fig. S1 Spin density plot for the most stable structures of seleno[n]helicenes radical cation, [n]SH$^{\bullet+}$, n=1-10 (S1a-S1j) at B3LYP-D/6-311++G(d,p) level of theory in DCM solvent with contour cutoff= 0.004 a.u.

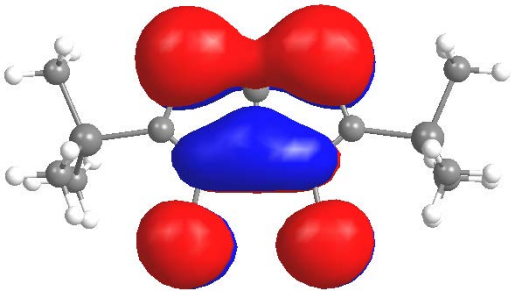
4) Molecular orbital plots with contour cutoff = 0.02 a.u. for the most stable structure of end substituted seleno[n]helicenes radical cation, n=2,4-6,8-10 (S2a-S2u) at B3LYP-D/6-311++G(d,p) level of theory in DCM solvent.



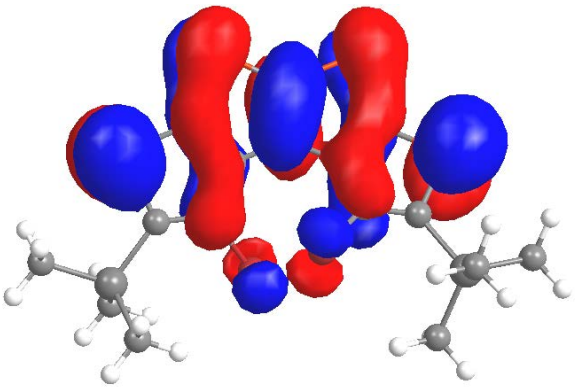
[2]SH$^{\bullet+}$ (H)
S2a



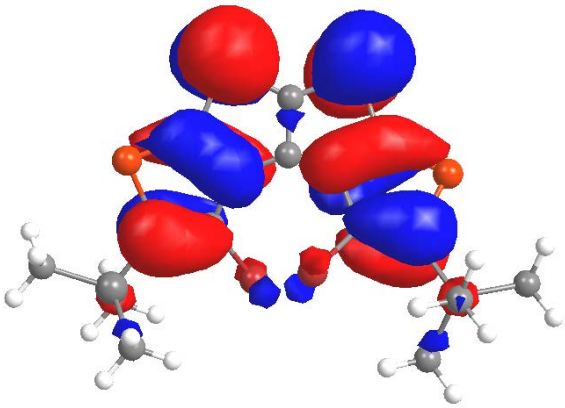
[2]SH$^{\bullet+}$ (L)
S2b



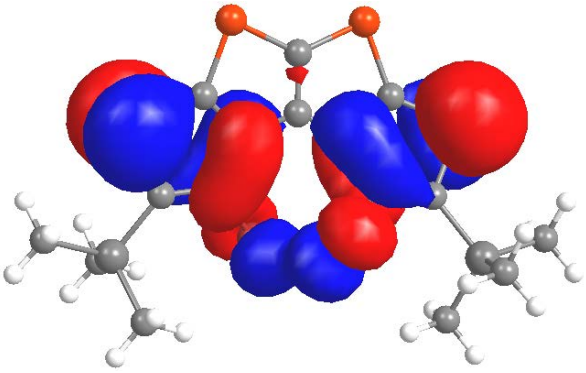
[2]SH$^{\bullet+}$ (H-1)
S2c



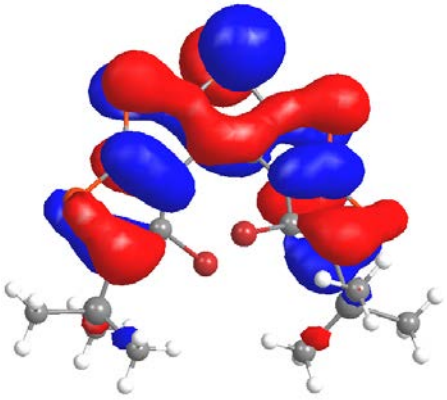
[4]SH$^{\bullet+}$ (H)
S2d



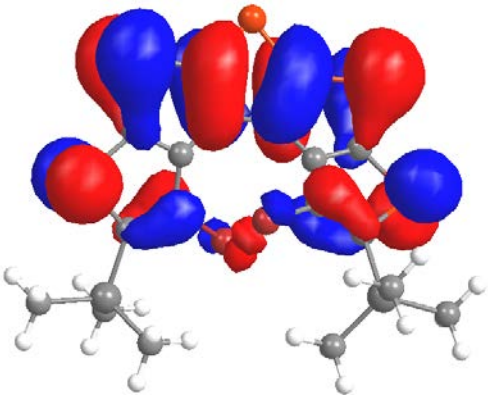
[4]SH$^{\bullet+}$ (L)
S2e



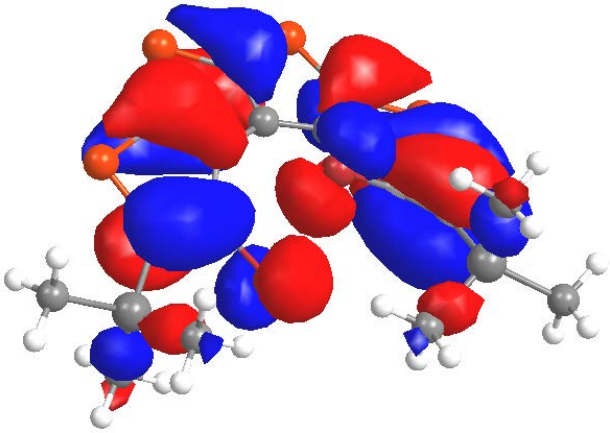
[4]SH$^{\bullet+}$ (H)
S2f



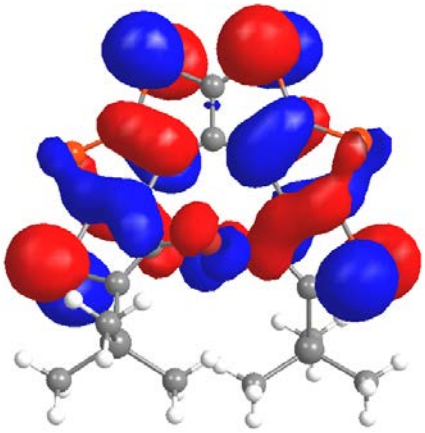
[5]SH$^{\bullet+}$ (H)
S2g



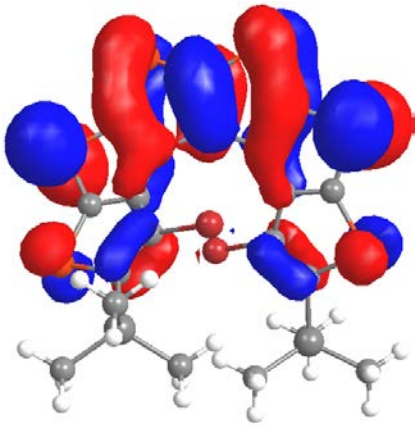
[5]SH$^{\bullet+}$ (L)
S2h



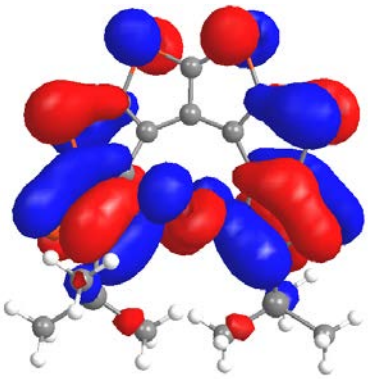
[5]SH$^{\bullet+}$ (H-1)
S2i



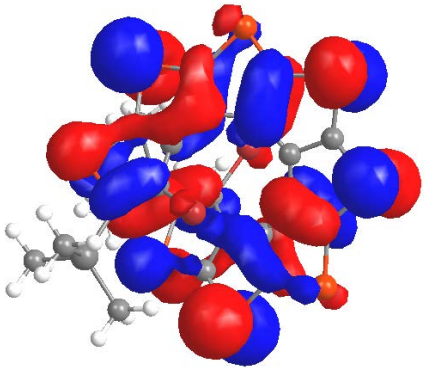
[6]SH$^{\bullet+}$ (H)
S2j



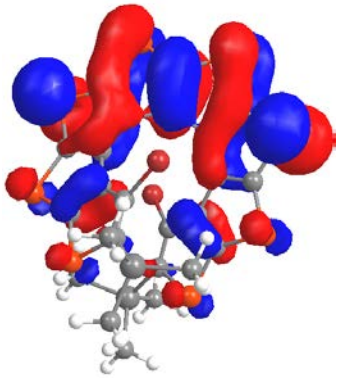
[6]SH$^{\bullet+}$ (L)
S2k



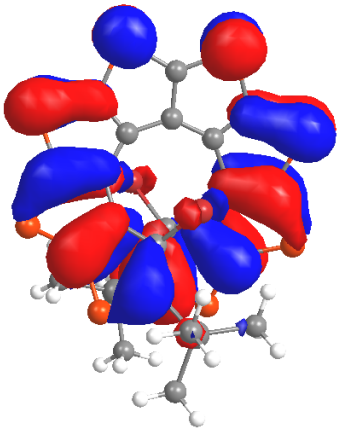
[6]SH$^{\bullet+}$ (H-1)
S2l



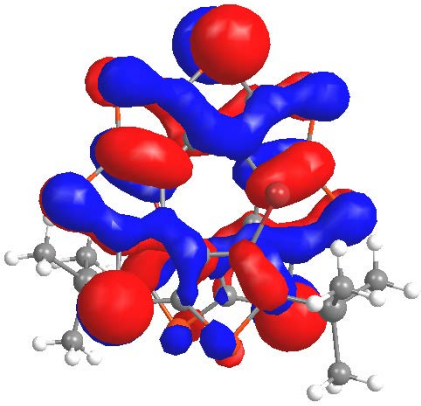
[8]SH$^{\bullet+}$ (H)
S2m



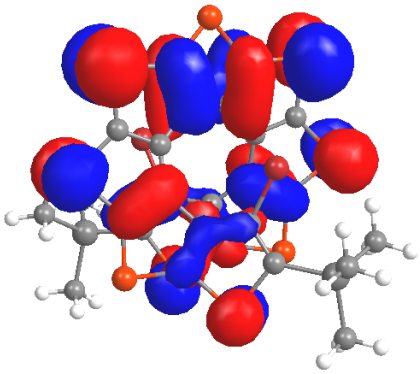
[8]SH$^{\bullet+}$ (L)
S2n



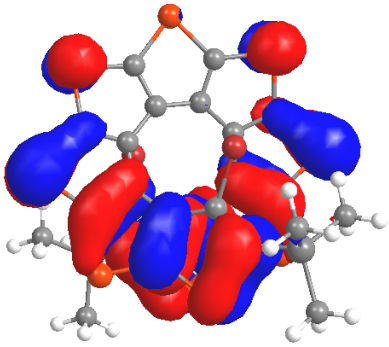
[8]SH$^{\bullet+}$ (H)
S2o



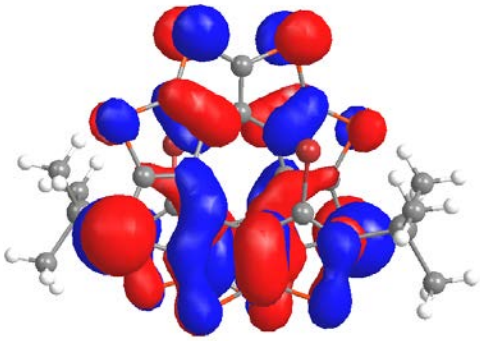
[9]SH$^{\bullet+}$ (H)
S2p



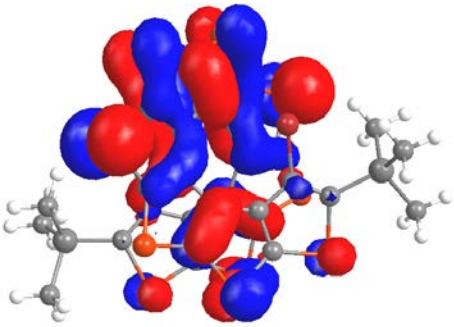
[9]SH$^{\bullet+}$ (L)
S2q



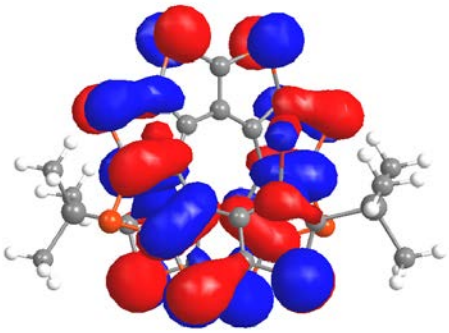
[9]SH$^{\bullet+}$ (H-2)
S2r



[10]SH$^{\bullet+}$ (H)
S2s



[10]SH$^{\bullet+}$ (L)
S2t



10]SH$^{\bullet+}$ (H-1)
S2u

Fig. S2 Molecular orbital plot for seleno[n]helicenes radical cation, [n]SH$^{\bullet+}$, n=2,4-6,8-10, S2a-S2u calculated using B3LYP-D as functional and 6-311++G(d,p) in DCM solvent with contour cutoff= 0.02 a.u.

5) Cartesian coordinates for the most stable structures of À-dimer of neutral unsubstituted and end substituted seleno[7]helicene at B3LYP-D /6-311++G(d,p) level in DCM solvent.

5.1 À-dimer of unsubstituted neutral seleno[7]helicene

C	0.000000	0.000000	0.000000
Se	0.000000	0.000000	1.890628
C	1.887743	0.000000	1.716438
Se	3.245532	-0.285044	2.999521
C	4.411041	-0.245542	1.512571
Se	6.221115	-0.773065	1.359456
C	5.975936	-0.434611	-0.483760
Se	7.180043	-0.554673	-1.933996
C	5.803913	0.287771	-2.914198
Se	5.801522	1.002728	-4.664979
C	4.190226	1.832010	-4.135838
Se	3.062355	3.082438	-4.970166
C	2.150901	3.159579	-3.306638
C	2.685607	2.325081	-2.380503
C	3.811697	1.550034	-2.832813
C	4.685309	0.606872	-2.161745
C	4.732124	0.079531	-0.809024
C	3.793914	0.031907	0.303624
C	2.344094	0.069341	0.411379
C	1.267326	-0.010441	-0.558300
C	1.265799	-0.251837	-1.974548
C	0.044140	-0.404556	-2.538491
Se	-1.360055	-0.258119	-1.273643
C	2.549296	-0.876431	-5.663576
C	3.097013	-1.669302	-4.712198
C	4.305068	-2.347471	-5.092634
C	5.243522	-3.155802	-4.336361
C	5.264329	-3.650867	-2.969065
C	4.291622	-3.686276	-1.885964
C	2.840760	-3.672350	-1.816380
C	1.795119	-3.921683	-2.789776
C	1.828726	-4.301592	-4.178266
C	0.615414	-4.504361	-4.749902
Se	-0.817334	-4.239171	-3.532970
C	0.515810	-3.878321	-2.258485
Se	0.467846	-3.614142	-0.389801
C	2.354109	-3.582044	-0.522375
Se	3.681364	-3.717006	0.813460
C	4.880106	-3.834867	-0.641451

Se	6.722819	-4.251573	-0.696171
C	6.527451	-4.053733	-2.567248
Se	7.824499	-4.060891	-3.941515
C	6.436453	-3.352334	-5.010354
Se	6.459392	-2.677341	-6.781717
C	4.721885	-2.050004	-6.379248
Se	3.552814	-0.876937	-7.271613
H	1.299407	3.815965	-3.192210
H	-0.187255	-0.586355	-3.578263
H	2.176165	-0.304107	-2.546899
H	2.289206	2.247302	-1.377413
H	0.404383	-4.776584	-5.774763
H	1.647471	-0.285141	-5.594261
H	2.657501	-1.787945	-3.736585
H	2.751958	-4.413859	-4.730007

5.2 À-dimer of unsubstituted radical cation of seleno[7]helicene

C	0.000000	0.000000	0.000000
Se	0.000000	0.000000	1.887777
C	1.871523	0.000000	1.716994
Se	3.217442	-0.285438	3.018623
C	4.384371	-0.258181	1.539626
Se	6.187448	-0.738697	1.411847
C	5.980799	-0.326850	-0.414770
Se	7.198247	-0.393097	-1.842993
C	5.831028	0.349387	-2.870830
Se	5.891730	1.129478	-4.594216
C	4.269454	1.927221	-4.085295
Se	3.169680	3.180683	-4.919029
C	2.200277	3.216917	-3.283415
C	2.696953	2.365347	-2.356567
C	3.841822	1.603433	-2.788654
C	4.685982	0.655226	-2.131677
C	4.722273	0.132589	-0.765316
C	3.774203	0.049686	0.313568
C	2.334712	0.075122	0.407079
C	1.264132	0.002436	-0.566482
C	1.252307	-0.189742	-1.990510
C	0.015518	-0.285887	-2.545641
Se	-1.365583	-0.197850	-1.270381
Se	6.283263	-3.285879	-2.554772
C	4.509589	-3.003233	-2.109818
Se	3.586560	-3.373908	-0.498767

C	2.059205	-3.290363	-1.577330
Se	0.272662	-3.636987	-1.177223
C	0.011050	-3.562903	-3.057038
Se	-1.468779	-3.922241	-4.134103
C	-0.280842	-3.729624	-5.595496
C	0.984727	-3.429313	-5.205816
C	1.161772	-3.308326	-3.783872
C	2.320997	-3.064669	-2.956609
C	3.682756	-2.778743	-3.225103
C	4.448916	-2.494383	-4.443384
C	5.784699	-2.836153	-4.312987
Se	6.839544	-2.500407	-5.835761
C	5.250749	-1.821492	-6.563259
Se	4.946281	-0.896106	-8.175057
C	3.255648	-0.494180	-7.422509
C	3.055973	-1.029417	-6.159400
C	4.159411	-1.833968	-5.686277
Se	1.838922	0.596897	-7.982908
C	1.073812	0.239552	-6.288459
C	1.839791	-0.587836	-5.536380
H	1.349103	3.876424	-3.186317
H	-0.240044	-0.413171	-3.586643
H	2.155260	-0.261809	-2.575230
H	2.269452	2.269306	-1.369085
H	-0.650912	-3.857754	-6.603148
H	0.125695	0.686731	-6.024718
H	1.564055	-0.887907	-4.540420
H	1.792233	-3.300984	-5.912245

5.3 À-dimer of end substituted neutral seleno[7]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.883213
C	1.774320	0.000000	2.519105
C	-0.821601	1.566283	2.549492
C	-2.114638	2.002891	2.490811
Br	-3.329745	1.090483	1.327360
Se	0.243965	2.880333	3.431718
C	-1.317291	3.893698	3.588113
C	-2.459496	3.262539	3.114013
C	-3.672056	4.070002	3.267650
C	-3.371519	5.359402	3.673102
Se	-1.574330	5.670840	4.151630
Se	-4.776464	6.603558	3.511134
C	-5.771282	5.106671	2.944951
C	-5.109685	3.888991	3.037699
C	-6.032576	2.763525	2.890926
C	-7.264070	3.157862	2.382218
Se	-7.548075	5.016744	2.331149
Se	-8.387102	1.754405	1.820828
C	-7.036730	0.650058	2.534212
Se	-6.884889	-1.235207	2.564867
C	-5.380621	-0.912377	3.657045
C	-5.142351	0.428062	3.914692
C	-5.997486	1.327905	3.150383
Se	-4.199201	-2.065471	4.534539
C	-3.475834	-0.517078	5.391860
Si	-2.078478	-0.714653	6.649662
C	-2.695685	-0.333485	8.386483
C	-4.142678	0.587055	4.943475
Br	-3.985459	2.242207	5.920236
C	-0.903313	-1.508355	2.550526
C	-1.510038	-2.509634	6.563714
C	-0.663455	0.422428	6.161122
Br	-5.927326	1.425553	-1.091610
C	-7.375979	2.507875	-1.718419
C	-8.545637	1.889950	-2.059271
Si	-8.970339	0.064003	-2.300293
C	-8.861604	-0.863300	-0.664752
C	-7.347582	3.951212	-1.617580
C	-6.348984	4.969454	-1.282634
C	-4.895372	5.014505	-1.088956
C	-3.743874	4.193532	-1.463232
C	-3.482239	3.104326	-2.398560

C	-4.165096	2.537664	-3.555165
C	-5.233816	2.962155	-4.427313
Br	-5.801572	4.804509	-4.468283
C	-8.624636	4.470328	-1.783796
Se	-8.790333	6.301528	-1.382641
C	-6.943924	6.191127	-1.016552
Se	-5.834383	7.463874	-0.181749
C	-4.508562	6.138170	-0.369947
Se	-2.721903	6.144156	0.221336
C	-2.599358	4.541843	-0.756373
Se	-1.167898	3.326657	-0.897139
C	-2.286528	2.454777	-2.138293
Se	-2.027858	0.848629	-3.103510
C	-3.627573	1.332899	-3.978896
Se	-4.581000	0.537464	-5.376640
C	-5.671084	2.108253	-5.399193
Si	-7.063064	2.259413	-6.669392
C	-7.223218	0.581527	-7.512869
Se	-9.918750	3.202428	-2.237931
C	-6.644405	3.570504	-7.953364
C	-8.660043	2.670502	-5.766854
C	-10.736728	-0.005586	-2.954289
C	-7.803300	-0.684264	-3.570954
H	-2.311163	-3.204810	6.841812
H	-1.160897	-2.775123	5.559331
H	-0.677508	-2.668439	7.260307
H	0.161260	0.335838	6.880125
H	-0.282039	0.157759	5.170523
H	-0.979164	1.468895	6.127843
H	-1.018912	0.055245	-0.392557
H	0.571277	0.846235	-0.398139
H	0.460782	-0.924126	-0.372361
H	-0.838385	-1.547254	3.642195
H	-1.961465	-1.501102	2.276224
H	-0.450867	-2.425227	2.151110
H	2.292523	-0.902988	2.173268
H	2.340153	0.865929	2.154973
H	1.809143	0.005411	3.614864
H	-3.015430	0.708857	8.481580
H	-3.544983	-0.975001	8.649772
H	-1.896377	-0.513352	9.116922
H	-11.453857	0.423555	-2.244247
H	-10.835180	0.530616	-3.905458
H	-11.027223	-1.049137	-3.127896
H	-8.023659	-1.751643	-3.701502

H	-7.921445	-0.193584	-4.541908
H	-6.757516	-0.585013	-3.268577
H	-6.563636	4.564911	-7.503497
H	-5.693158	3.343292	-8.449016
H	-7.426761	3.606271	-8.722405
H	-8.918544	1.875511	-5.061176
H	-8.576294	3.603144	-5.202014
H	-9.486081	2.775745	-6.481835
H	-8.041387	0.610412	-8.243166
H	-6.308431	0.307281	-8.051724
H	-7.446338	-0.213381	-6.792089
H	-7.857663	-0.790687	-0.237942
H	-9.577656	-0.468514	0.064930
H	-9.090257	-1.925302	-0.822394

5.4 À-dimer of end substituted radical cation of seleno[7]helicene

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.882240
C	1.768860	0.000000	2.523885
C	-0.815579	1.594357	2.522140
C	-2.102642	2.049369	2.424242
Br	-3.327557	1.112190	1.301182
Se	0.237124	2.888472	3.433327
C	-1.295872	3.927719	3.546755
C	-2.430152	3.324553	3.022439
C	-3.622405	4.154800	3.142809
C	-3.289915	5.476332	3.565461
Se	-1.541313	5.690674	4.183035
Se	-4.696559	6.712765	3.547069
C	-5.697761	5.239153	2.922053
C	-5.032523	3.995120	2.976797
C	-5.971165	2.881850	2.806100
C	-7.182967	3.302245	2.275891
Se	-7.418719	5.163466	2.255002
Se	-8.390493	1.934600	1.843842
C	-7.074278	0.807154	2.544416
Se	-6.978461	-1.073579	2.627755
C	-5.444506	-0.762429	3.688665
C	-5.157893	0.577032	3.907758
C	-5.983628	1.473173	3.124356
Se	-4.273289	-1.918555	4.559981
C	-3.488308	-0.375446	5.370694
Si	-2.108566	-0.600339	6.654604

C	-2.762723	-0.190639	8.368847
C	-4.129327	0.737674	4.909876
Br	-3.930900	2.406715	5.853696
C	-0.933115	-1.476159	2.572780
C	-1.584030	-2.406357	6.576522
C	-0.665590	0.507099	6.182795
Se	-2.686889	6.082515	0.516000
C	-2.608726	4.491375	-0.475135
Se	-1.170594	3.321708	-0.756080
C	-2.311221	2.517282	-1.999578
Se	-2.095053	0.965481	-3.047678
C	-3.707504	1.518803	-3.865736
Se	-4.708538	0.802978	-5.263272
C	-5.777587	2.386378	-5.195313
Si	-7.159129	2.630813	-6.473719
C	-7.370306	0.986644	-7.365379
C	-4.425661	6.203096	-0.095936
C	-4.875283	5.075753	-0.817103
C	-3.756701	4.209911	-1.202600
C	-3.523842	3.193936	-2.202264
C	-4.223927	2.708677	-3.374012
C	-5.310704	3.189771	-4.195872
Br	-5.829474	5.045722	-4.148909
Se	-5.687439	7.595946	0.084372
C	-6.866780	6.332157	-0.636606
Se	-8.653645	6.538890	-1.135952
C	-8.570577	4.688853	-1.514932
C	-7.328039	4.101149	-1.325194
C	-6.298467	5.059811	-0.942815
Se	-9.901094	3.501346	-2.027315
C	-8.605127	2.119932	-1.867932
Si	-9.111588	0.314232	-2.183510
C	-9.023308	-0.658713	-0.574650
C	-7.409184	2.666582	-1.488476
Br	-5.993385	1.504107	-0.955394
C	-6.664003	3.970373	-7.696338
C	-8.743019	3.075182	-5.565380
C	-10.883601	0.350148	-2.815348
C	-7.978033	-0.412367	-3.492593
H	-2.405075	-3.082597	6.842374
H	-1.224539	-2.679877	5.577842
H	-0.766820	-2.583849	7.286358
H	0.160572	0.367751	6.891514
H	-0.299962	0.263186	5.181069
H	-0.945197	1.564193	6.190940

H	-1.015163	0.054684	-0.403315
H	0.576799	0.843961	-0.395822
H	0.461849	-0.924966	-0.368060
H	-0.903391	-1.473842	3.666421
H	-1.980991	-1.483353	2.261621
H	-0.465921	-2.405774	2.223569
H	2.285872	-0.901680	2.173608
H	2.336332	0.866994	2.164719
H	1.802300	-0.001831	3.619619
H	-3.056754	0.860385	8.450748
H	-3.634671	-0.808504	8.613173
H	-1.988206	-0.386552	9.121193
H	-11.570559	0.798039	-2.087209
H	-10.967457	0.908922	-3.754759
H	-11.225705	-0.674404	-3.005824
H	-8.266684	-1.451304	-3.696791
H	-8.058329	0.150007	-4.427584
H	-6.930415	-0.404605	-3.180580
H	-6.553914	4.944212	-7.209174
H	-5.713544	3.723711	-8.183711
H	-7.429411	4.065368	-8.476983
H	-9.014964	2.291154	-4.852649
H	-8.644681	4.013406	-5.012432
H	-9.566835	3.186616	-6.281720
H	-8.178143	1.068437	-8.102883
H	-6.460953	0.692986	-7.902902
H	-7.632751	0.180859	-6.670224
H	-8.013853	-0.651287	-0.153741
H	-9.714100	-0.251410	0.172712
H	-9.305844	-1.702826	-0.759943

5.5 À-dimer of unsubstituted of seleno[7]helicene radical cation with two PF_6^- counter ions

C	0.000000	0.000000	0.000000
Se	0.000000	0.000000	1.897323
C	1.871367	0.000000	1.732316
Se	3.232982	-0.177090	3.015371
C	4.389183	-0.010466	1.528468
Se	6.225249	-0.177096	1.375346
C	5.985517	0.285704	-0.422972
Se	7.258864	0.688073	-1.746082
C	5.806302	1.385460	-2.683032
Se	5.727414	2.294502	-4.327908
C	3.947983	2.690999	-3.817212
Se	2.662072	3.837224	-4.540776
C	1.684097	3.531329	-2.942007
C	2.318112	2.684100	-2.097748
C	3.577890	2.175079	-2.579128
C	4.588747	1.349345	-1.977662
C	4.679419	0.609578	-0.748595
C	3.741516	0.277376	0.314637
C	2.329604	0.144887	0.406625
C	1.262480	0.058789	-0.563195
C	1.269051	-0.075274	-1.991847
C	0.044312	-0.218317	-2.557760
Se	-1.352461	-0.199311	-1.280857
F	3.184988	3.083606	0.915881
P	4.386572	4.149891	1.257134
F	5.410137	3.324417	0.274002
F	5.587520	5.221835	1.608570
F	4.855251	3.211983	2.528475
F	3.365543	4.979531	2.248758
F	3.919207	5.086530	-0.011024
C	4.338118	-1.385053	-3.402405
C	3.708666	-0.907777	-4.503859
Se	4.763676	-1.052794	-6.064232
C	6.071137	-1.791282	-4.951005
Se	7.873970	-2.259782	-5.249531
C	7.883421	-2.657455	-3.405960
Se	9.290181	-3.191563	-2.292068
C	7.997597	-3.187486	-0.940191
Se	8.178592	-3.571218	0.903299
C	6.344221	-3.275325	0.970183
Se	5.130659	-3.465843	2.408290
C	3.824876	-3.242650	1.066029
Se	1.972424	-3.254989	1.162270

C	2.024052	-3.440535	-0.724619
Se	0.722248	-3.914716	-1.974693
C	2.160999	-4.204765	-3.160451
C	3.369704	-3.936933	-2.597869
C	3.306843	-3.476227	-1.240751
C	4.333684	-3.221543	-0.250880
C	5.741893	-3.081221	-0.304226
C	6.709865	-2.899734	-1.362772
C	6.655996	-2.496016	-2.761047
C	5.653659	-1.926367	-3.631420
F	5.784724	-5.993791	-0.556182
P	6.262834	-6.866339	-1.863522
F	6.742899	-7.747371	-3.169419
F	6.204574	-5.516041	-2.796926
F	4.689500	-7.185505	-2.225672
F	6.324361	-8.223990	-0.932220
F	7.836476	-6.548012	-1.500482
H	0.735039	4.027362	-2.794859
H	-0.193037	-0.322709	-3.607061
H	2.179810	-0.049429	-2.566927
H	1.927000	2.441598	-1.122130
H	1.964068	-4.541058	-4.168704
H	2.722178	-0.474243	-4.572694
H	3.895128	-1.345119	-2.421233
H	4.301916	-4.093354	-3.118670

5.6 À-dimer of end substituted of seleno[7]helicene radical cation with two PF_6^- counter ions

C	0.000000	0.000000	0.000000
Si	0.000000	0.000000	1.881129
C	1.759800	0.000000	2.546348
C	-0.799289	1.612131	2.476018
C	-2.095195	2.051437	2.409787
Br	-3.380236	1.075938	1.385205
Se	0.296016	2.999078	3.167293
C	-1.235774	4.042011	3.265183
C	-2.392155	3.370484	2.901699
C	-3.588214	4.193641	2.985536
C	-3.261292	5.556522	3.166092
Se	-1.475501	5.890272	3.570328
Se	-4.700878	6.748495	2.959750
C	-5.710390	5.169769	2.723372

C	-5.006843	3.977088	2.942873
C	-5.896209	2.820279	3.006131
C	-7.154482	3.105582	2.494644
Se	-7.479511	4.936472	2.185871
Se	-8.302692	1.622357	2.334043
C	-6.895562	0.680328	3.137934
Se	-6.722401	-1.158489	3.510350
C	-5.106068	-0.646520	4.335950
C	-4.864188	0.720153	4.336920
C	-5.805691	1.466271	3.521220
Se	-3.814602	-1.630874	5.249124
C	-3.037761	0.037334	5.767097
Si	-1.554960	0.016816	6.946737
C	-2.109534	0.550652	8.663020
C	-3.767627	1.052840	5.218999
Br	-3.587452	2.834775	5.930988
C	-0.939953	-1.460485	2.601978
C	-0.927494	-1.758517	6.980402
C	-0.204858	1.138986	6.282424
F	-0.232388	4.499888	0.230863
P	0.918748	5.585252	-0.240586
F	1.644805	5.449045	1.227891
F	2.065198	6.663816	-0.709853
F	1.834526	4.348141	-0.814743
F	0.181822	5.725875	-1.702635
F	-0.009859	6.814996	0.339337
Se	-3.095141	5.384152	-0.129695
C	-4.748844	5.825454	-0.835638
Se	-5.911274	7.241451	-0.417349
C	-7.016003	6.452312	-1.727839
Se	-8.550809	7.103661	-2.535696
C	-8.519451	5.509237	-3.529776
Se	-9.643962	4.926373	-4.920482
C	-8.637726	3.353344	-4.829835
Se	-8.733062	1.798685	-5.879127
C	-7.499210	1.110123	-4.628713
Se	-6.766940	-0.581456	-4.426396
C	-6.050548	0.010857	-2.765764
Si	-5.068094	-1.236833	-1.730795
C	-5.224329	-2.913134	-2.575258
C	-5.181545	5.000479	-1.908588
C	-6.536725	5.244453	-2.279243
C	-7.512078	4.622904	-3.176238
C	-7.685584	3.322604	-3.795872
C	-7.150912	1.990041	-3.609476

C	-6.405179	1.318658	-2.568396
Br	-6.240516	2.115939	-0.832891
C	-4.114224	4.124872	-2.369873
C	-3.855022	3.370882	-3.568747
Br	-4.812220	3.736032	-5.191799
C	-3.032797	4.084697	-1.505851
Se	-1.702105	2.905742	-2.039217
C	-2.711587	2.610424	-3.614690
Si	-1.977510	1.501388	-4.972700
C	-1.362704	2.583833	-6.381889
C	-5.772607	-1.368965	0.005885
C	-3.261069	-0.720067	-1.728519
C	-0.527735	0.595158	-4.184052
C	-3.289403	0.291738	-5.551947
F	-7.686310	-0.772729	-7.484765
P	-8.889814	-1.893165	-7.625726
F	-7.923101	-3.013924	-6.910490
F	-8.311824	-2.329055	-9.099847
F	-10.091385	-3.005224	-7.759488
F	-9.462397	-1.447929	-6.147200
F	-9.851046	-0.761604	-8.333502
H	-1.677409	-2.457429	7.369354
H	-0.635430	-2.091783	5.977357
H	-0.044084	-1.827676	7.626902
H	0.646596	1.144264	6.975080
H	0.151193	0.784156	5.310522
H	-0.549329	2.169179	6.159222
H	-1.013411	0.083940	-0.399331
H	0.589122	0.843170	-0.378346
H	0.444370	-0.926182	-0.385858
H	-0.925692	-1.423876	3.696943
H	-1.983948	-1.481551	2.277903
H	-0.465784	-2.399454	2.288643
H	2.273504	-0.922001	2.247911
H	2.343535	0.843995	2.159988
H	1.768773	0.049087	3.641846
H	-2.465819	1.586005	8.666020
H	-2.920393	-0.089054	9.030604
H	-1.272848	0.477307	9.369316
H	0.259271	1.291374	-3.870293
H	-0.833597	0.010002	-3.310245
H	-0.085130	-0.094769	-4.912987
H	-2.858976	-0.402876	-6.284392
H	-3.679338	-0.294375	-4.715757
H	-4.132979	0.801018	-6.026602

H	-5.744622	-0.430730	0.561060
H	-6.817620	-1.698639	-0.030403
H	-5.204665	-2.116106	0.573045
H	-2.823230	-0.890722	-2.716926
H	-3.129142	0.334499	-1.478176
H	-2.696648	-1.318472	-1.004464
H	-4.635120	-3.652481	-2.018233
H	-6.261905	-3.265089	-2.602013
H	-4.842969	-2.896204	-3.602966
H	-2.182853	3.121647	-6.868004
H	-0.637135	3.321401	-6.019607
H	-0.867194	1.963987	-7.139982