Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

A simple construction of multiple highly-efficient orange-emitting carboranes based on interlocked molecular aggregations

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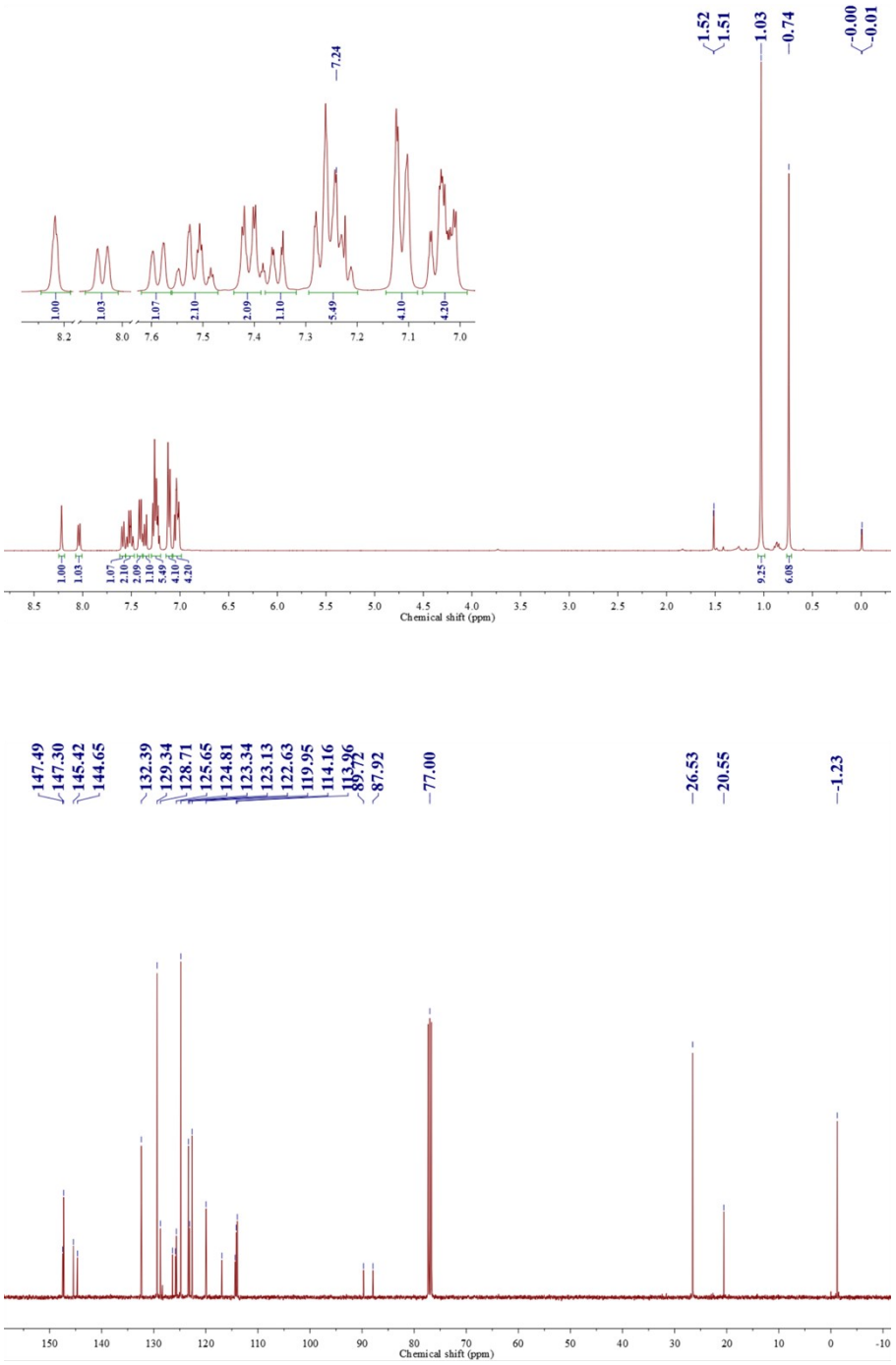


Figure S1. ^{1}H and ^{13}C NMR spectra of **TPA-C≡C-CzSi**.

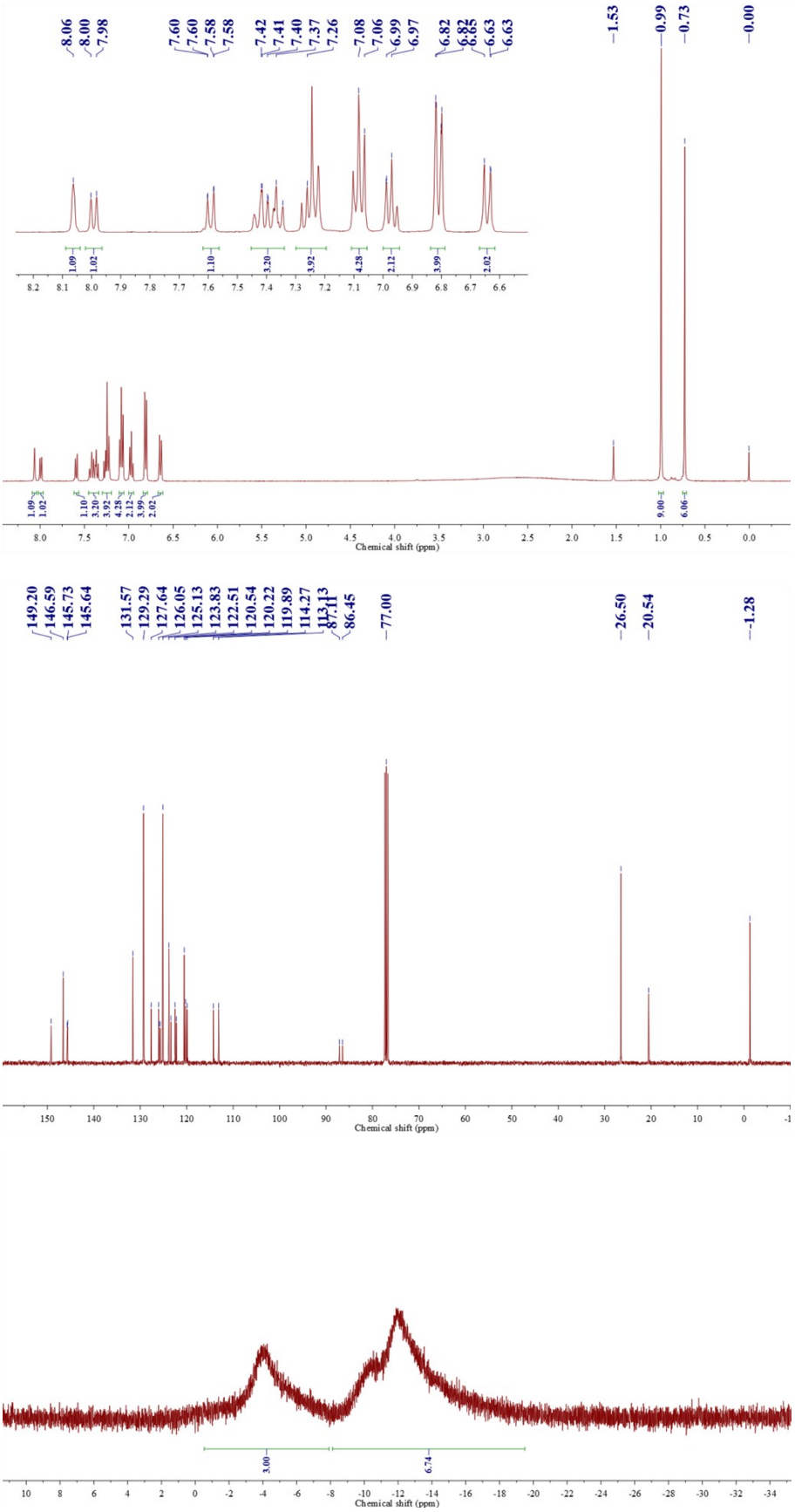


Figure S2. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-Si**.

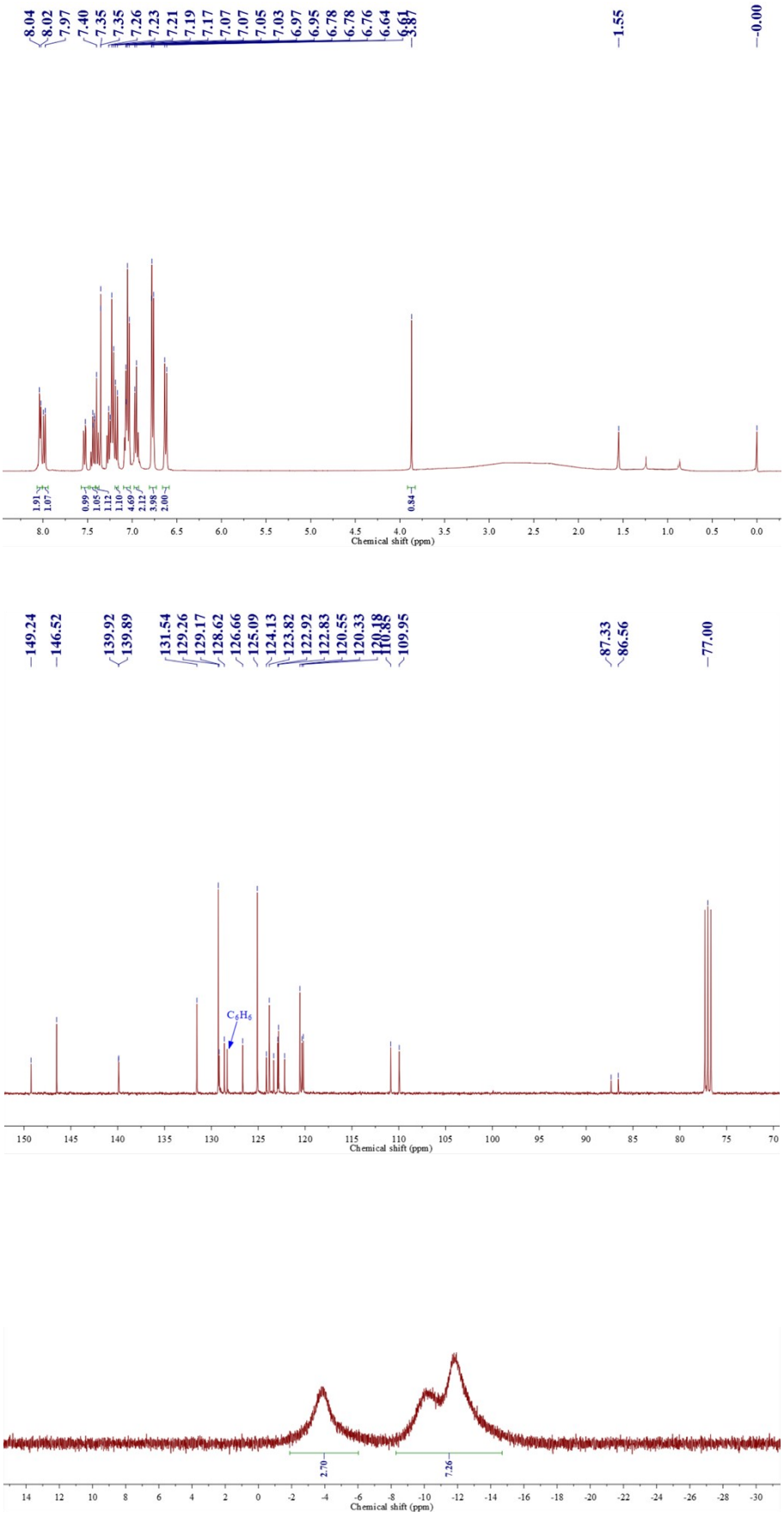


Figure S3. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-H**.

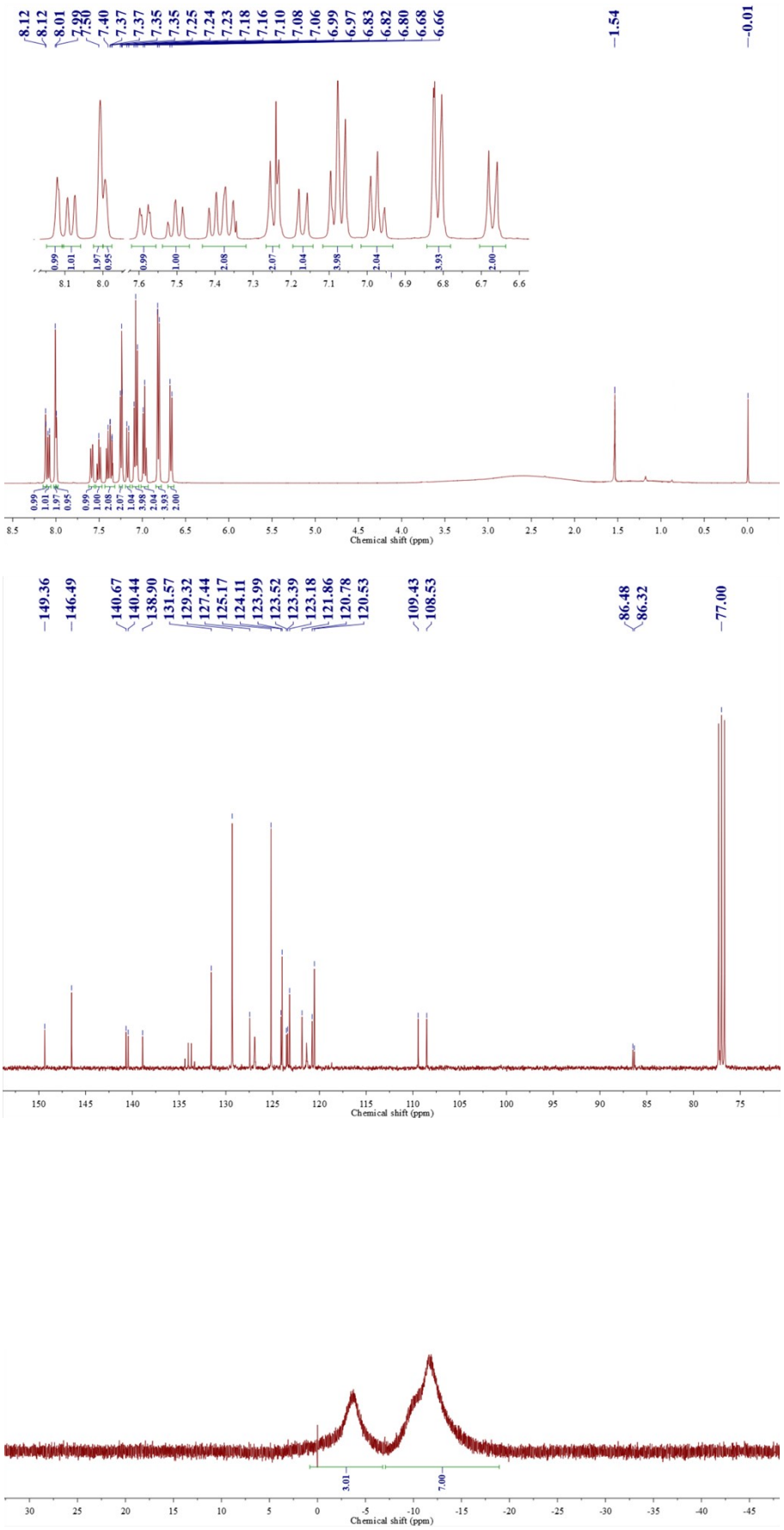


Figure S4. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-CF_3**.

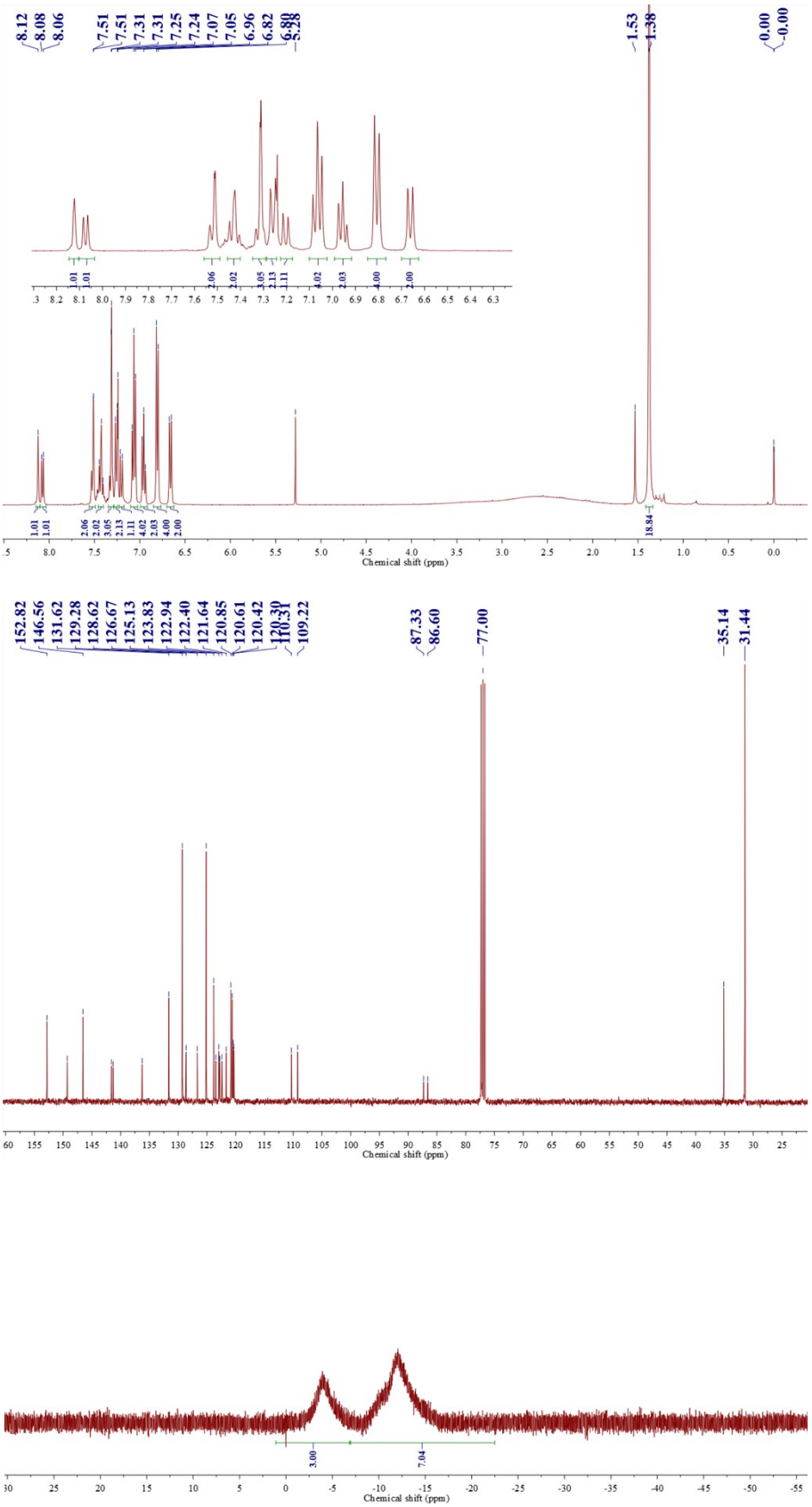


Figure S5. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-Bu**.

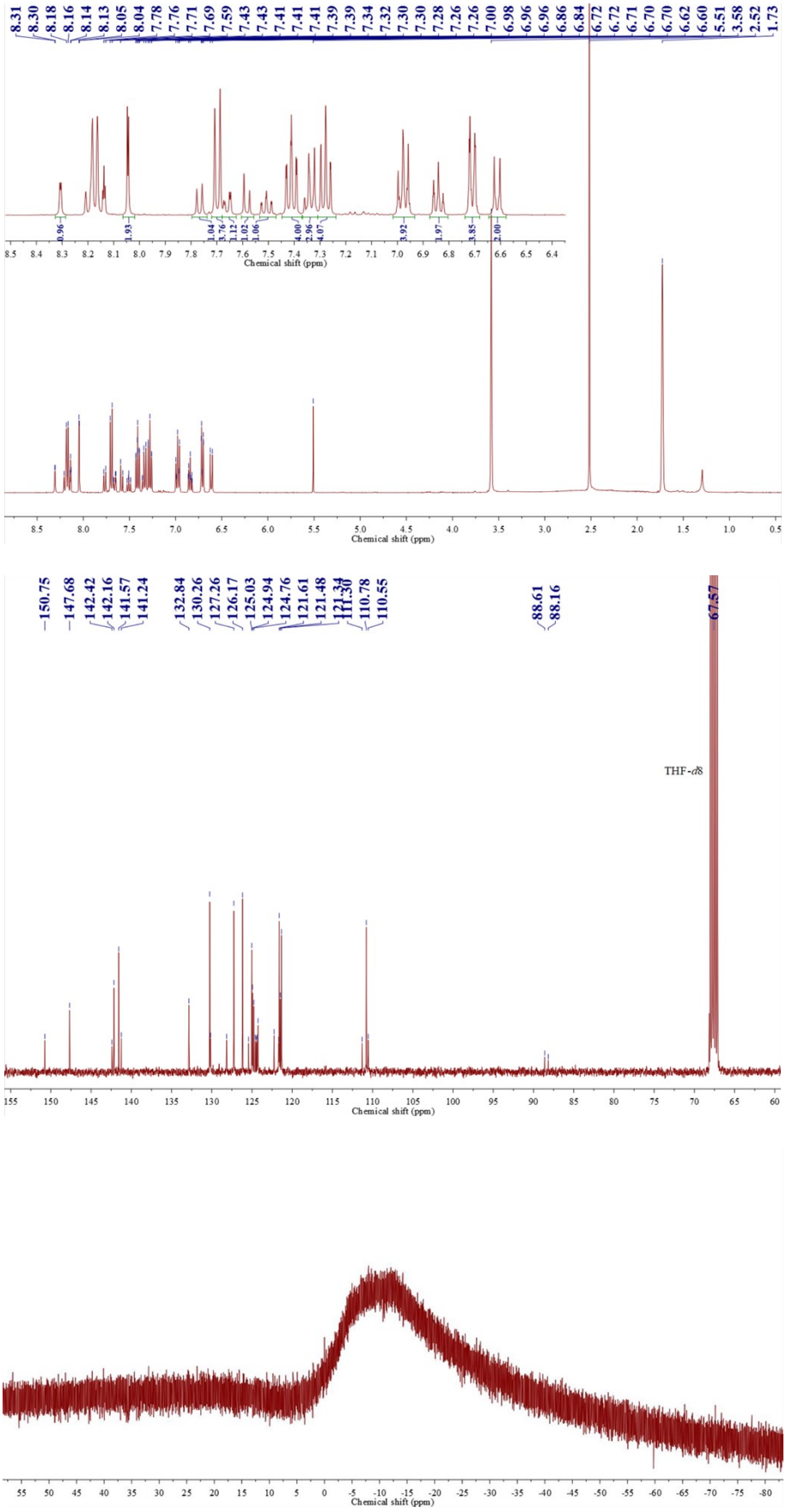


Figure S6. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-Cz** (in THF-d8, poorly dissolved)

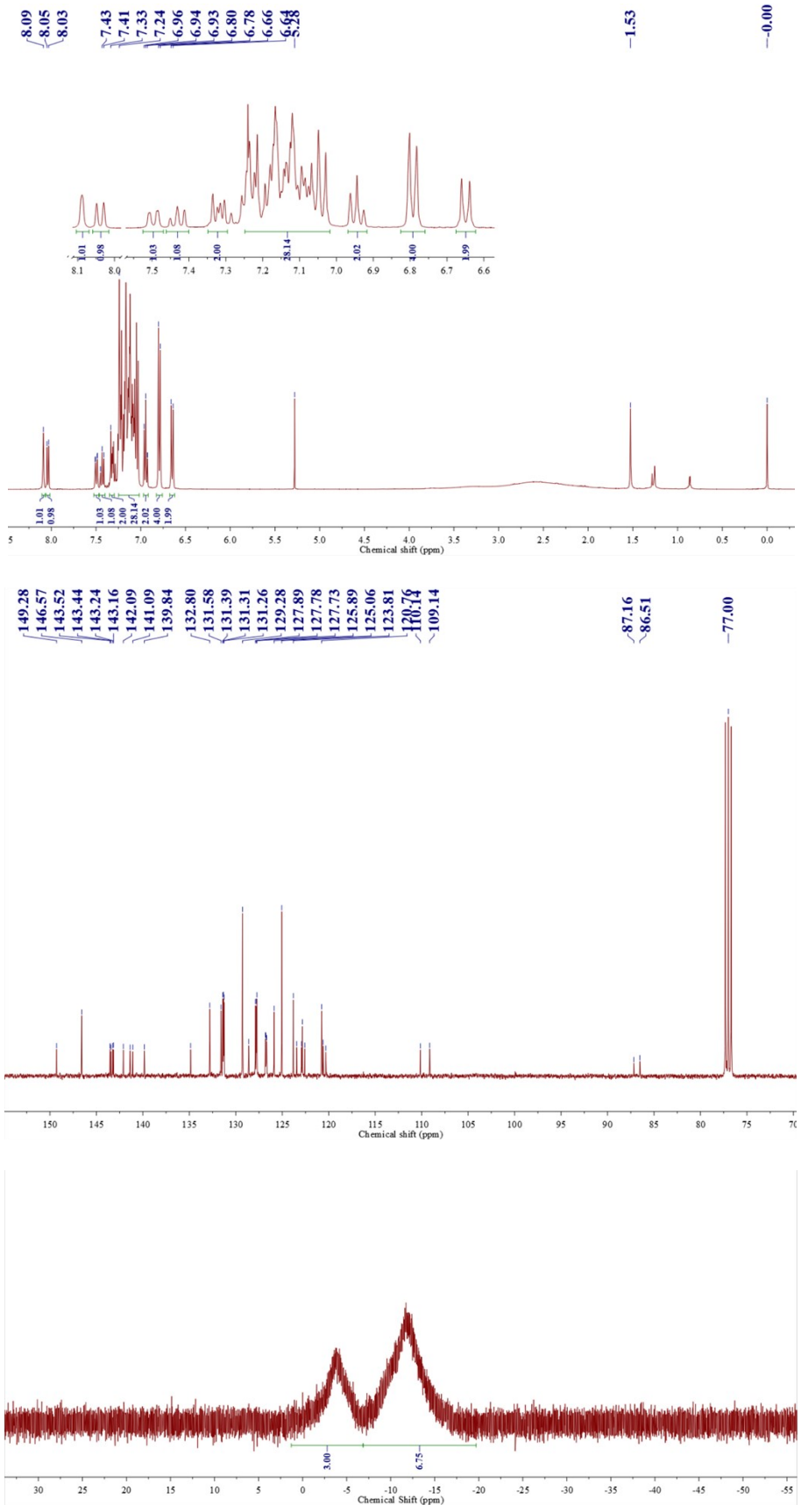


Figure S7. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-TPE**.

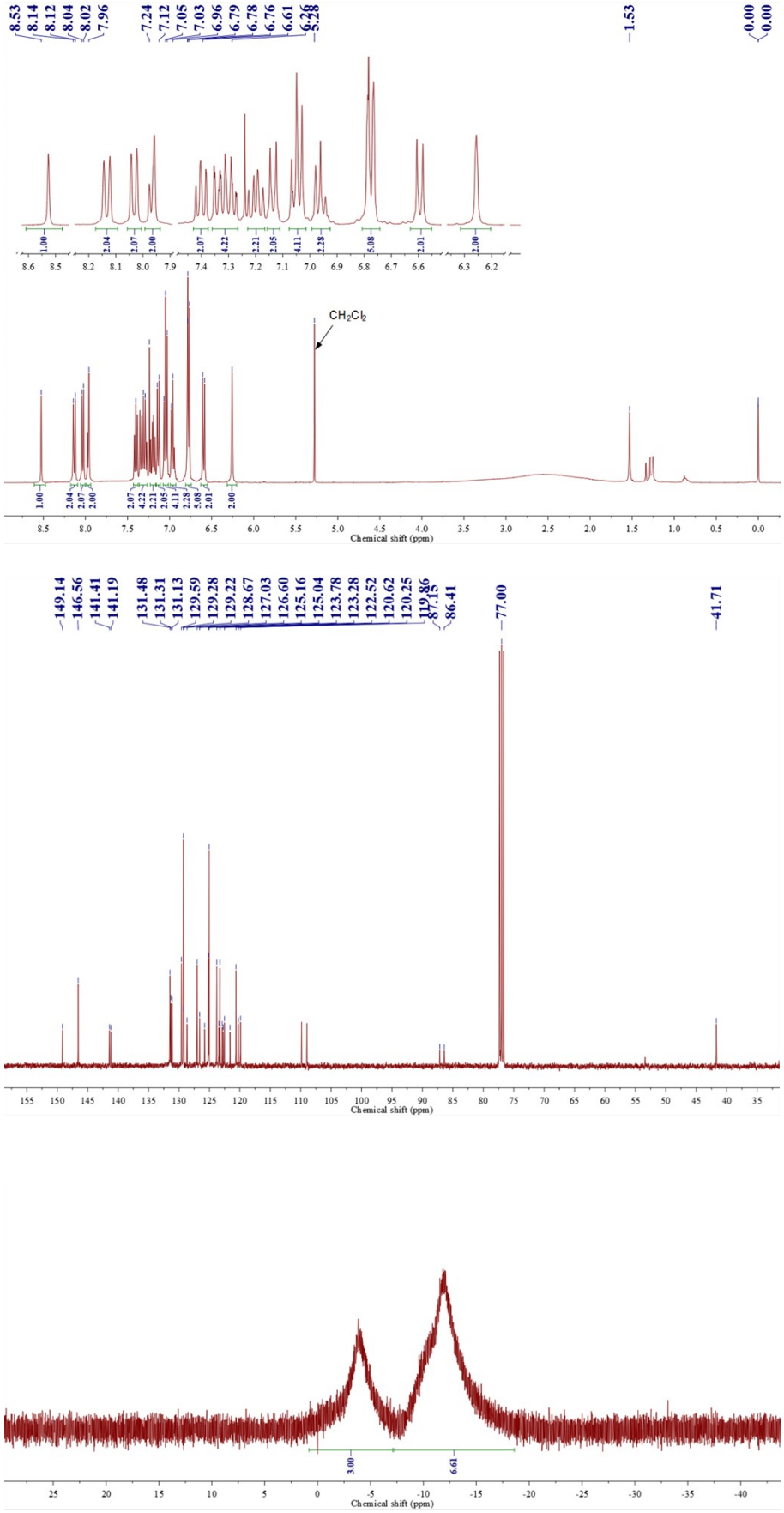


Figure S8. ^{1}H, ^{13}C and ^{11}B NMR spectra of **CB-An**.

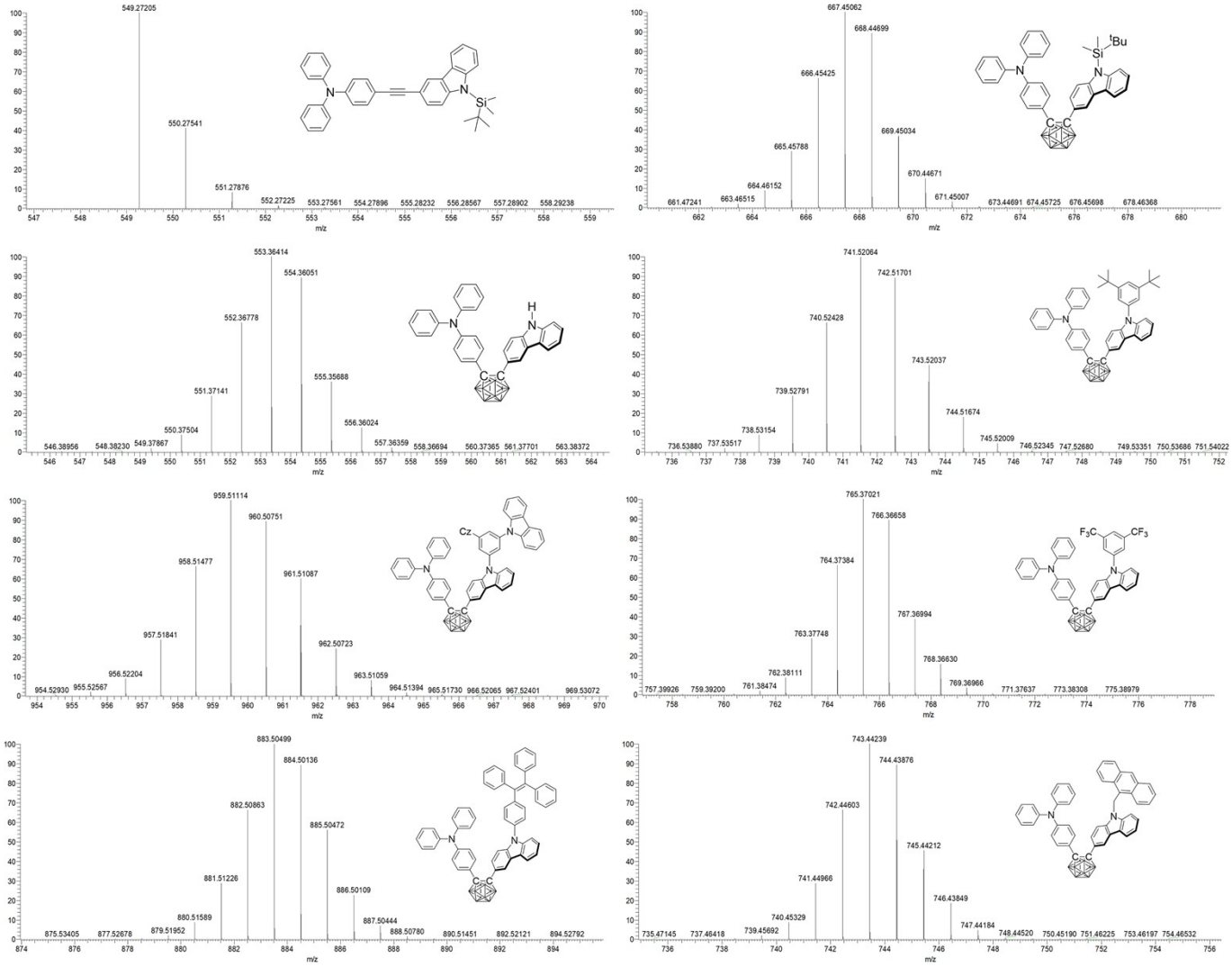


Figure S9. HRMS spectra of the synthesized compounds.

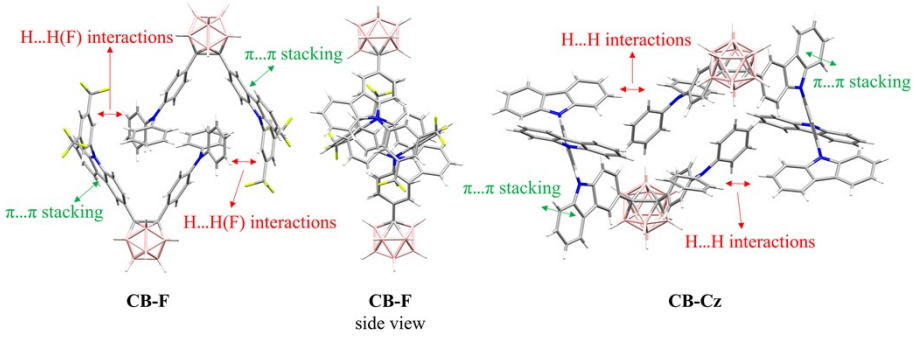


Figure S10. An analysis of intermolecular interactions and vibrations along carboranyl C–C bonds in the two crystals.

Table S1. Crystallographic data of **CB-Cz** and **CB-CF_3**

Crystals	**CB-CF_3**	**CB-Cz**
CCDC number	2111386	2111387
Empirical formula	$C_{40}H_{34}B_{10}F_6N_2$	$C_{62}H_{50}B_{10}N_4 \cdot C_7H_8$
Formula weight (g/mol)	764.79	1051.29
Temperature (K)	273	273
Wavelength (Å)	1.54178	1.54178
Crystal system	Triclinic	Triclinic
Space group	P -1	P -1
Unit cell dimensions	a = 11.9655 Å b = 13.7759 Å c = 16.4271 Å α = 75.949˚ β = 70.772˚ γ = 64.736˚	a = 13.6658 Å b = 15.1862 Å c = 15.5361 Å α = 96.143˚ β = 103.721˚ γ = 111.943˚
Volume (Å3)	2295.5	2836.0
Z	2	2
Dx, g/cm3	1.107	1.231
Mu (mm-1)	0.642	0.518
F000	784.0	1100.0
F000’	786.50	1102.74
h, k, l max	13, 16, 19	15, 17, 18
N_{ref}	7626	9357
R(reflections)	0.0927	0.0603
wR2(reflections)	0.3029	0.1623
S(GOOF)	1.050	1.064

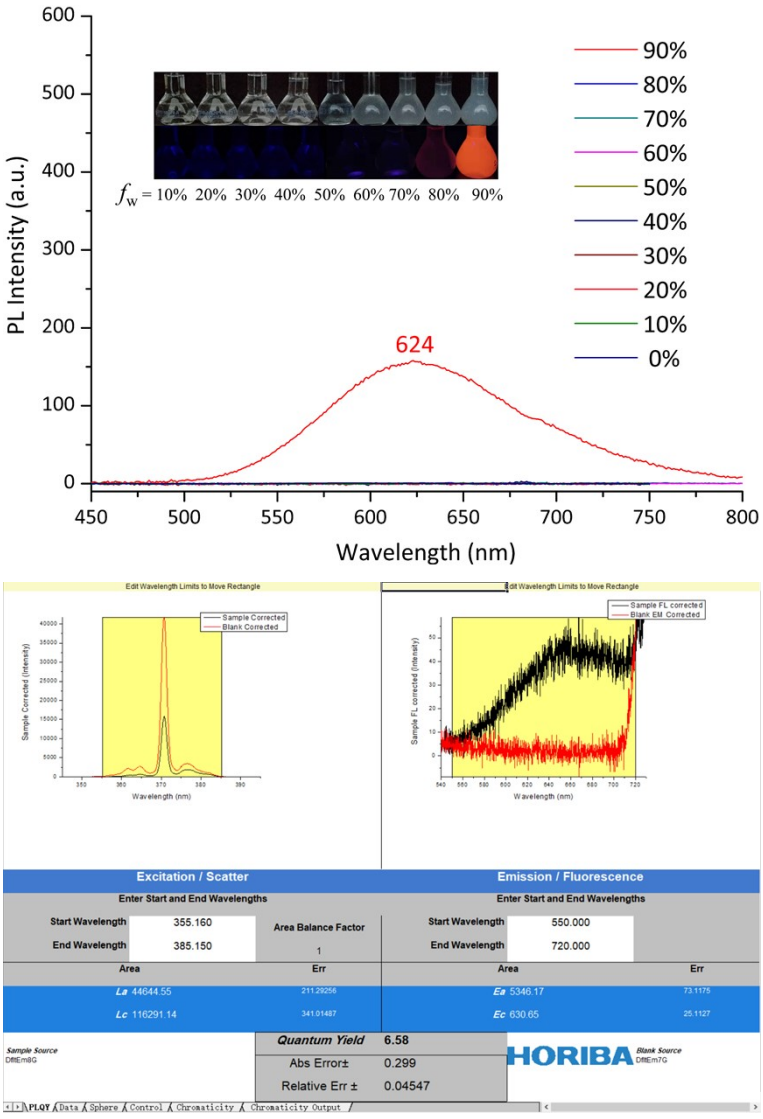


Figure S11. (up) PL appearance of **CB-H** in different ratios of THF/water under the irradiation of 365 nm. The concentrations were controlled at 0.1 g/L; (down) PL efficiency evaluation of **CB-H** aggregates in THF/water (f_w = 90%).

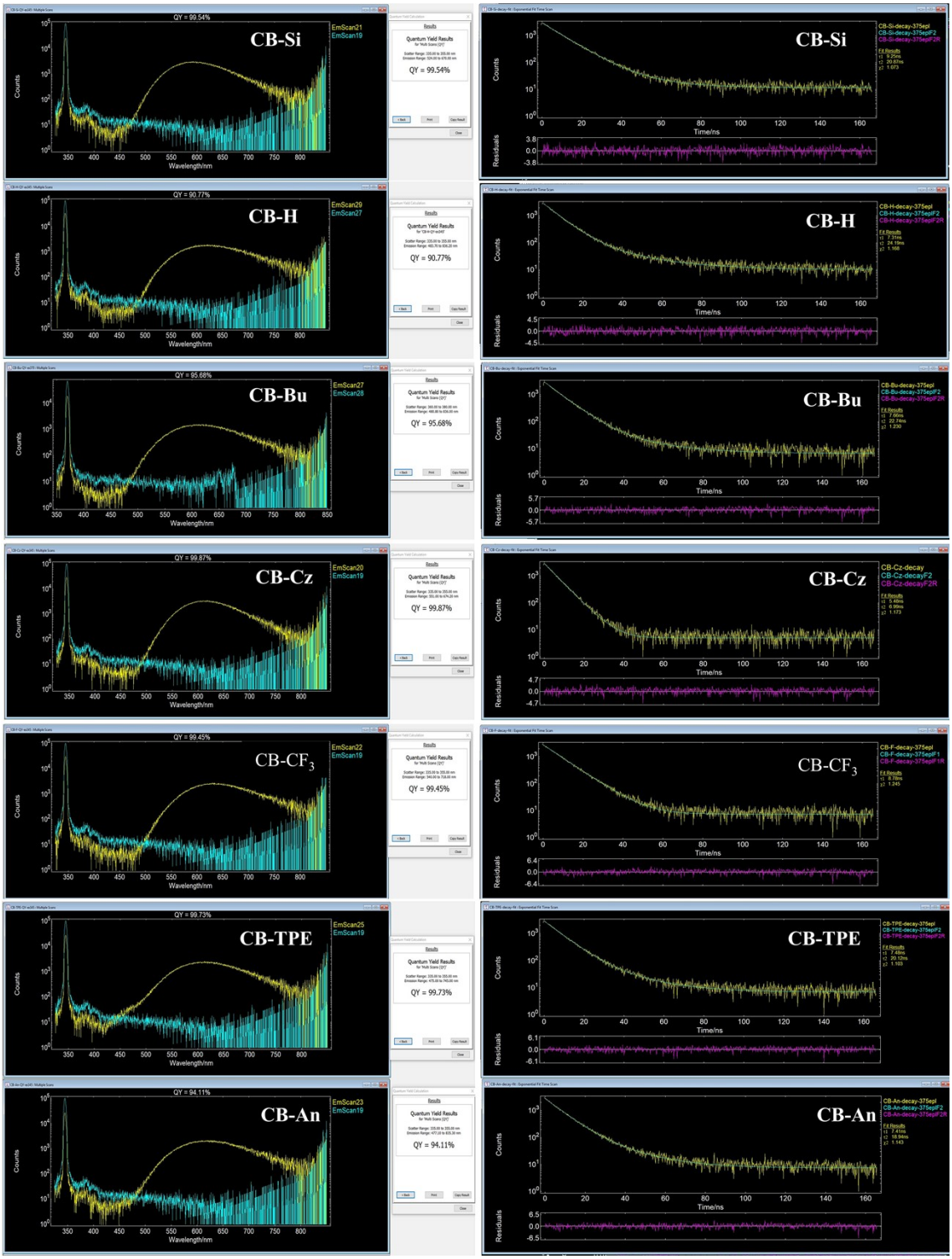


Figure S12. Evaluations of quantum efficiencies and PL decay curves of the carboranes. All the data were provided by Shiyanjia Lab (www.shiyanjia.com)

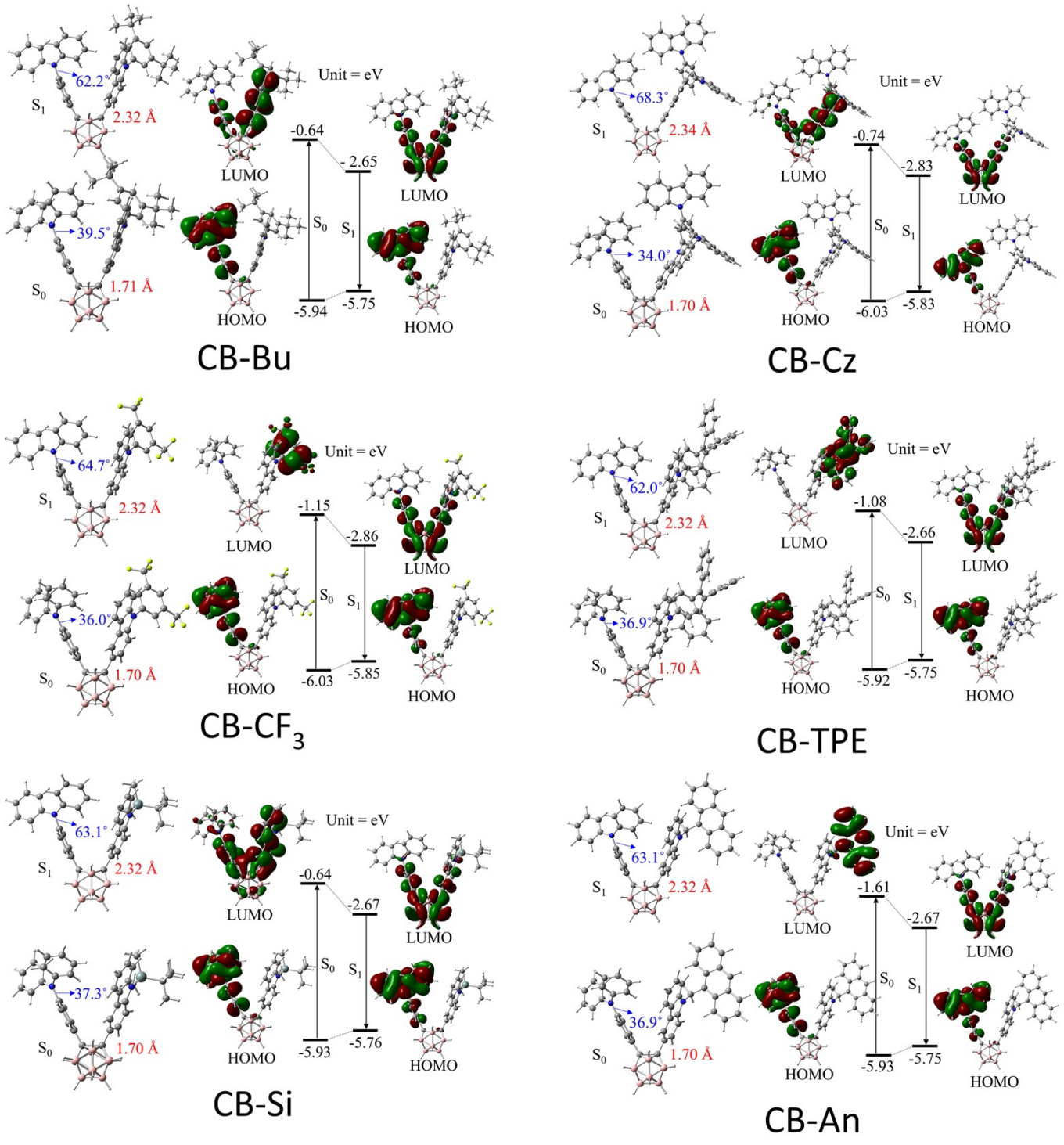


Figure S13. Optimized structures and electronic transitions of the derived carboranes (free) at the ground (S_0) and first excited (S_1) state.

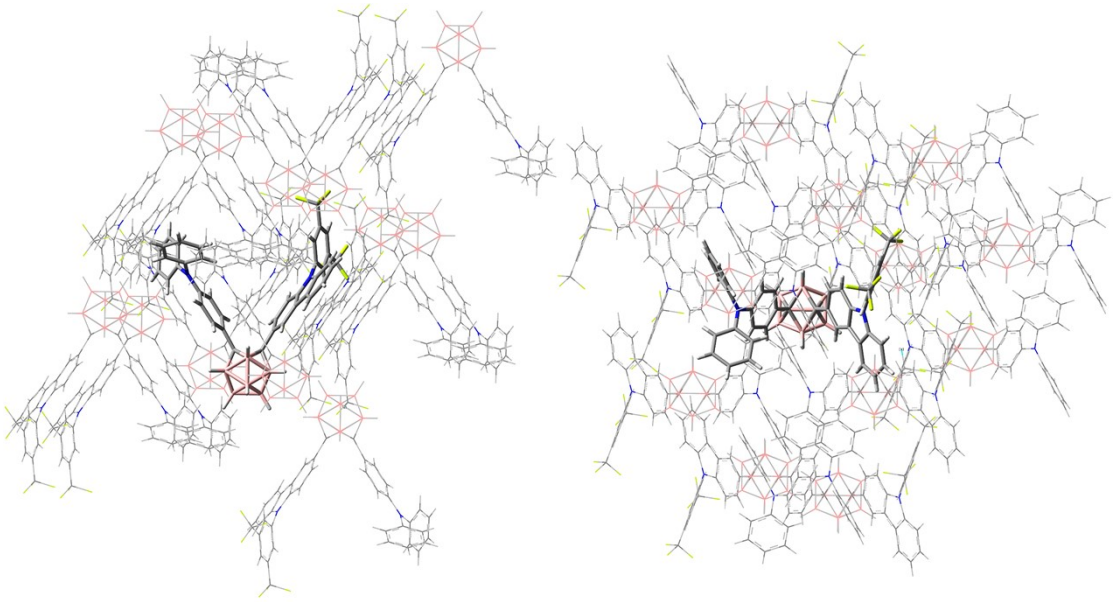
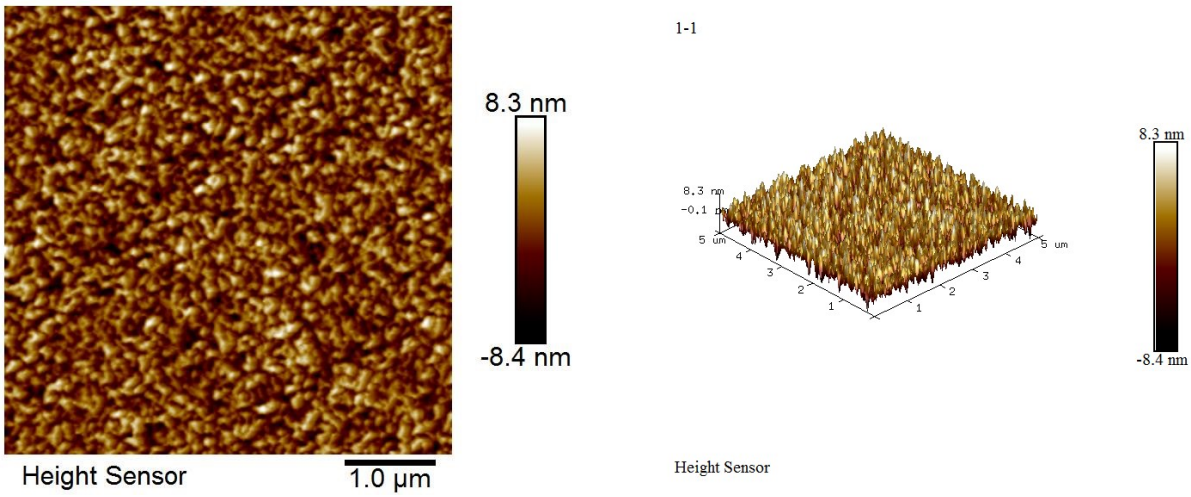


Figure S14. Different views of the selected cluster from **CB-CF$_3$** crystal for the ONIOM modelling.



Figre S15. Atomic force microscopy of the vapor-deposited film of **CB-Bu** (30 nm).

Table S2. Coordinates of the optimized structures of carboranes in the ground and first excited states

	CB-H at S_0				**CB-H** at S_1		
C	-1.539976	2.829597	1.928173	C	-1.927946	2.9051	1.691488
C	-2.897008	0.754845	0.679114	C	-3.124329	0.61424	0.645646
C	-3.639837	-0.388821	0.059783	C	-3.691815	-0.644778	0.158432
C	-3.023282	0.983416	2.059538	C	-3.170484	0.913372	2.025628
H	-3.662004	0.336681	2.643691	H	-3.679997	0.221399	2.682127
C	-1.244532	-1.655531	-0.424968	C	-0.827495	-2.21528	-0.320699
C	-0.110904	4.396416	1.19285	C	-0.716828	4.566425	0.786123
C	-2.080296	1.586043	-0.07628	C	-2.478213	1.506578	-0.207882
H	-1.969507	1.430522	-1.138613	H	-2.436713	1.297771	-1.267434
C	-2.361858	2.014177	2.696058	C	-2.59273	2.045193	2.559689
H	-2.482263	2.170451	3.759884	H	-2.649582	2.245739	3.622014

C	-1.392423	2.620433	0.543259	C	-1.871022	2.644642	0.311008
C	-0.472327	3.626044	0.069706	C	-1.094261	3.713041	-0.274399
C	-0.496153	-1.275653	-1.538914	C	-0.114509	-1.872502	-1.479629
C	-2.735328	-1.719658	-0.500656	C	-2.276295	-2.409214	-0.373745
C	-0.55434	-1.988769	0.738264	C	-0.120385	-2.289786	0.887493
C	0.822915	-1.899522	0.806189	C	1.216435	-1.946986	0.955227
C	0.773541	5.463422	1.096691	C	0.061259	5.698746	0.57196
H	1.04582	6.050446	1.964245	H	0.344142	6.349779	1.389498
C	0.067968	3.93531	-1.175559	C	-0.686772	4.014873	-1.570581
H	-0.199089	3.356142	-2.050437	H	-0.975165	3.376636	-2.396367
C	1.295348	5.750758	-0.152247	C	0.45566	5.973207	-0.72764
H	1.98496	6.57821	-0.258332	H	1.05382	6.854389	-0.922641
C	0.8805	-1.191012	-1.483483	C	1.219843	-1.523842	-1.423094
C	0.948625	4.997864	-1.278762	C	0.087268	5.142827	-1.79055
H	1.369276	5.25562	-2.241878	H	0.402547	5.390886	-2.795598
B	-3.511144	-0.6738	-1.614872	B	-3.188309	-1.321916	-1.333897
H	-2.855624	0.047316	-2.27605	H	-2.586845	-0.634115	-2.094774
B	-3.510681	-2.423861	-1.835821	B	-3.087355	-3.139623	-1.575423
H	-2.814035	-2.878421	-2.677457	H	-2.439794	-3.621598	-2.449092
B	-5.118466	-0.930452	0.701034	B	-4.945569	-1.445686	0.800499
H	-5.565745	-0.335214	1.620157	H	-5.526668	-0.922453	1.695461
B	-3.593548	-3.16632	-0.238903	B	-3.13219	-3.703157	0.119661
H	-2.948302	-4.124843	0.016131	H	-2.517134	-4.618438	0.564103
B	-5.041328	-0.190279	-0.893163	B	-4.907	-0.887276	-0.896837
H	-5.410073	0.920168	-1.067015	H	-5.440743	0.081089	-1.329962
B	-4.990293	-1.48796	-2.095752	B	-4.603254	-2.30142	-1.905448
H	-5.421404	-1.324704	-3.188	H	-5.013725	-2.298152	-3.020706
B	-3.636683	-1.857119	0.941313	B	-3.244523	-2.095846	0.992205
H	-3.069311	-1.871804	1.974455	H	-2.708912	-1.958974	2.045207
B	-5.05517	-3.039104	-1.231017	B	-4.59236	-3.770206	-0.888462
H	-5.546207	-4.008165	-1.706254	H	-5.022207	-4.81829	-1.248772
B	-5.122203	-2.689235	0.509596	B	-4.673082	-3.191608	0.80076
H	-5.658145	-3.386266	1.30497	H	-5.148981	-3.832644	1.681088
B	-5.998637	-1.660065	-0.645446	B	-5.666216	-2.441019	-0.479788
H	-7.183137	-1.618653	-0.681805	H	-6.846976	-2.561091	-0.545487
H	-0.994388	-1.058826	-2.473442	H	-0.635259	-1.846344	-2.426241
H	1.438267	-0.895936	-2.361598	H	1.750477	-1.223032	-2.317643
H	1.331242	-2.143657	1.728698	H	1.741603	-1.963032	1.901868
H	-1.096569	-2.309161	1.615491	H	-0.644053	-2.583051	1.785619
N	-0.766798	3.898996	2.295726	N	-1.229676	4.062788	1.954905
C	1.564467	-1.48134	-0.300435	C	1.87543	-1.536158	-0.197526
N	2.954442	-1.351301	-0.234454	N	3.222797	-1.052379	-0.113129
C	3.596348	-0.298431	-0.924061	C	3.447347	0.284352	-0.387086
C	4.776714	-0.537979	-1.625547	C	4.680459	0.718916	-0.914607
C	3.064058	0.990259	-0.901154	C	2.408596	1.217254	-0.194253
C	5.414469	0.499071	-2.287181	C	4.868476	2.052415	-1.205209
H	5.188365	-1.538509	-1.644045	H	5.451985	-0.004182	-1.138327
C	3.698872	2.017507	-1.580788	C	2.618013	2.547884	-0.484274

H	2.152531	1.183915	-0.350665	H	1.45768	0.885087	0.195813
C	4.878225	1.779464	-2.273342	C	3.846075	2.97319	-0.986498
H	6.330963	0.29984	-2.82794	H	5.808361	2.37626	-1.631365
H	3.269985	3.01128	-1.550591	H	1.819362	3.260139	-0.326654
H	5.376456	2.584914	-2.796851	H	3.996321	4.017371	-1.224059
C	3.720672	-2.222503	0.567475	C	4.224692	-1.932675	0.256719
C	4.755587	-1.725447	1.358656	C	5.353432	-1.491504	0.972147
C	3.459568	-3.592617	0.56946	C	4.083712	-3.300035	-0.039068
C	5.515991	-2.587547	2.132135	C	6.326615	-2.395129	1.343564
H	4.959322	-0.662902	1.359087	H	5.427368	-0.454664	1.268223
C	4.212982	-4.444018	1.361085	C	5.071527	-4.186201	0.332901
H	2.664416	-3.982792	-0.052166	H	3.207738	-3.63685	-0.57396
C	5.247422	-3.949154	2.143305	C	6.198091	-3.742664	1.020649
H	6.317066	-2.18732	2.740557	H	7.181599	-2.052606	1.910493
H	3.997872	-5.504984	1.352776	H	4.965312	-5.233433	0.085317
H	5.839253	-4.618278	2.753788	H	6.963443	-4.446343	1.318159
H	-0.688785	4.26229	3.225284	H	-1.150635	4.49566	2.853704

	CB-Si at S_0				**CB-Si** at S_1		
C	-2.523503	0.287893	-0.178382	C	-2.609572	0.532676	-0.200847
C	-0.910171	2.555973	0.124091	C	-0.884565	2.731294	0.114855
C	-0.04632	3.774782	0.222428	C	0.077371	3.832273	0.194454
C	-1.708987	2.370074	-1.013861	C	-1.611051	2.515927	-1.074775
H	-1.703019	3.121222	-1.790734	H	-1.487645	3.220932	-1.885637
C	2.183637	2.174446	0.039698	C	2.795565	1.976387	-0.022587
C	-2.909915	-1.474234	1.139382	C	-3.166985	-1.16085	1.152038
C	-0.942628	1.598399	1.127263	C	-1.071288	1.836179	1.164567
H	-0.352914	1.716989	2.023715	H	-0.543144	1.98297	2.096081
C	-2.518772	1.263159	-1.17327	C	-2.471294	1.451294	-1.241963
H	-3.132721	1.180894	-2.055834	H	-3.015741	1.351591	-2.167739
C	-1.739069	0.472225	0.975312	C	-1.918147	0.746487	1.003041
C	-1.984694	-0.662107	1.822355	C	-2.27718	-0.339321	1.875642
C	2.636507	1.517507	1.183608	C	3.173155	1.296441	1.145662
C	1.641226	3.563776	0.130087	C	2.346514	3.366279	0.042514
C	2.271553	1.498891	-1.175302	C	2.793716	1.260085	-1.228079
C	2.742179	0.201304	-1.242347	C	3.06386	-0.094408	-1.254364
C	-3.388623	-2.639639	1.733863	C	-3.711784	-2.295058	1.752675
H	-4.124145	-3.262597	1.249955	H	-4.419764	-2.924515	1.236988
C	-1.513837	-1.025147	3.080569	C	-1.923568	-0.657559	3.183143
H	-0.802228	-0.39666	3.601226	H	-1.246205	-0.017094	3.734118
C	-2.911294	-2.984424	2.986582	C	-3.344166	-2.598082	3.054379
H	-3.280534	-3.886689	3.457133	H	-3.771673	-3.472799	3.528386
C	3.115842	0.224333	1.125646	C	3.440286	-0.057392	1.131827
C	-1.97745	-2.192452	3.658357	C	-2.455027	-1.793145	3.769017
H	-1.630543	-2.486217	4.640379	H	-2.196026	-2.049646	4.787954
B	0.909637	4.024465	1.610178	B	1.338966	3.816614	1.354212
H	0.862074	3.245442	2.492103	H	1.261913	3.057945	2.26631
B	2.42313	4.746331	1.062547	B	2.990313	4.525052	0.97951

H	3.423321	4.421558	1.605264	H	3.955417	4.234002	1.61097
B	-0.484352	5.230998	-0.538161	B	0.000726	5.238432	-0.607392
H	-1.524927	5.263189	-1.099533	H	-0.977233	5.449501	-1.248782
B	2.353652	4.871256	-0.694751	B	2.90742	4.639908	-0.802259
H	3.30348	4.624857	-1.356076	H	3.805312	4.43417	-1.553976
B	-0.416188	5.111889	1.215906	B	0.085904	5.131874	1.17445
H	-1.405813	5.035725	1.859423	H	-0.824906	5.240232	1.928647
B	1.143231	5.75908	1.746945	B	1.729761	5.562585	1.645867
H	1.266501	6.251881	2.818184	H	1.902675	6.039769	2.720419
B	0.79694	4.216057	-1.201454	B	1.227835	3.96937	-1.092949
H	0.633059	3.550582	-2.160464	H	1.010669	3.325363	-2.068843
B	2.032556	6.297016	0.305635	B	2.649079	6.080078	0.204023
H	2.805297	7.19588	0.338188	H	3.459657	6.949381	0.222781
B	1.022714	5.955801	-1.115835	B	1.590183	5.740064	-1.195203
H	1.046712	6.595506	-2.11383	H	1.643784	6.355541	-2.210446
B	0.27858	6.520698	0.397	B	0.93204	6.437142	0.311464
H	-0.238455	7.583988	0.487837	H	0.540109	7.556115	0.396605
H	2.630852	2.029227	2.135797	H	3.217657	1.841676	2.077668
H	3.461682	-0.263547	2.026567	H	3.693387	-0.579796	2.045757
H	2.778669	-0.307461	-2.195718	H	3.013933	-0.647804	-2.183594
H	1.952114	1.982046	-2.086731	H	2.537191	1.77291	-2.143549
N	-3.225459	-0.910299	-0.100167	N	-3.365554	-0.643262	-0.127958
C	3.155212	-0.466237	-0.087938	C	3.357594	-0.756209	-0.067353
N	3.594477	-1.792706	-0.135079	N	3.509117	-2.181104	-0.065336
C	3.268266	-2.67865	0.915942	C	2.572782	-2.930147	0.624288
C	4.225613	-3.564437	1.407719	C	2.916834	-4.17227	1.195109
C	1.98615	-2.684143	1.464545	C	1.27334	-2.417606	0.810914
C	3.899539	-4.444366	2.427185	C	1.97316	-4.885431	1.901586
H	5.220918	-3.558468	0.983221	H	3.933022	-4.532884	1.120573
C	1.674347	-3.554726	2.496591	C	0.341157	-3.148605	1.515076
H	1.236107	-2.004049	1.081983	H	1.010436	-1.459497	0.386826
C	2.626299	-4.4418	2.980391	C	0.682892	-4.384361	2.060146
H	4.652243	-5.127618	2.79963	H	2.24942	-5.826845	2.356932
H	0.673491	-3.542756	2.909693	H	-0.656617	-2.752566	1.648421
H	2.37829	-5.126158	3.781136	H	-0.051362	-4.944357	2.622868
C	4.302488	-2.275048	-1.255081	C	4.564358	-2.739989	-0.765947
C	4.00865	-3.528828	-1.789917	C	4.450931	-4.009572	-1.361804
C	5.312909	-1.507652	-1.834535	C	5.749341	-2.001587	-0.930566
C	4.718526	-4.004064	-2.880767	C	5.512568	-4.532407	-2.06993
H	3.225064	-4.125732	-1.342502	H	3.515422	-4.547409	-1.300587
C	6.003818	-1.983442	-2.936959	C	6.802364	-2.544815	-1.634767
H	5.551128	-0.539089	-1.414966	H	5.826618	-1.020985	-0.483998
C	5.715208	-3.234557	-3.464461	C	6.694738	-3.81063	-2.204485
H	4.479992	-4.980007	-3.2842	H	5.411633	-5.500327	-2.541859
H	6.784803	-1.375762	-3.376042	H	7.717437	-1.978599	-1.741379
H	6.262835	-3.606549	-4.320268	H	7.521945	-4.225352	-2.76413
Si	-4.246563	-1.643891	-1.386998	Si	-4.374247	-1.345045	-1.432914
C	-4.092666	-3.514878	-1.302236	C	-4.366623	-3.221688	-1.284779

H	-3.08696	-3.821558	-1.012333	H	-3.397142	-3.594548	-0.952048
H	-4.800294	-3.989614	-0.62325	H	-5.130372	-3.618368	-0.616398
H	-4.285221	-3.917352	-2.298627	H	-4.558706	-3.640737	-2.274465
C	-3.578095	-1.132798	-3.067346	C	-3.598695	-0.953696	-3.100019
H	-3.858873	-1.899977	-3.791571	H	-3.889877	-1.734083	-3.80584
H	-3.973009	-0.186456	-3.435612	H	-3.919004	-0.002322	-3.5234
H	-2.489364	-1.067821	-3.063472	H	-2.509589	-0.946417	-3.043931
C	-6.041908	-1.077589	-1.149518	C	-6.137284	-0.654609	-1.306387
C	-6.561127	-1.527638	0.216477	C	-6.744372	-1.008412	0.051713
H	-5.968522	-1.113189	1.034354	H	-6.16186	-0.595505	0.877466
H	-7.593451	-1.191092	0.354674	H	-7.757324	-0.600491	0.12719
H	-6.56253	-2.615334	0.318268	H	-6.821624	-2.088121	0.200105
C	-6.128805	0.446628	-1.23425	C	-6.117581	0.866966	-1.458305
H	-5.522262	0.932365	-0.467397	H	-5.510117	1.346153	-0.688402
H	-5.807803	0.82417	-2.207782	H	-5.732769	1.179134	-2.431727
H	-7.163746	0.772143	-1.089613	H	-7.13344	1.265316	-1.37197
C	-6.901092	-1.700155	-2.252254	C	-6.987431	-1.268101	-2.420954
H	-6.882646	-2.792183	-2.219398	H	-7.047651	-2.356224	-2.339848
H	-7.944512	-1.390255	-2.137534	H	-8.010536	-0.882362	-2.370521
H	-6.578961	-1.388205	-3.248613	H	-6.599404	-1.025477	-3.413169

CB-An at S_0

C	1.489664	-1.020242	-0.415966	C	-1.569405	1.11747	-0.378933
C	-0.648669	-2.784258	-0.126479	C	0.544272	2.931204	-0.105428
C	-1.791971	-3.745724	-0.027322	C	1.696399	3.832517	-0.037407
C	0.114301	-2.747613	-1.30355	C	-0.17125	2.799463	-1.314272
H	-0.135137	-3.416632	-2.114566	H	0.123183	3.414185	-2.153821
C	-3.553834	-1.629581	-0.038861	C	4.033068	1.501585	-0.108749
C	2.357032	0.559586	0.914444	C	-2.463893	-0.41422	0.993458
C	-0.329614	-1.918817	0.912125	C	0.165676	2.137272	0.976175
H	-0.901702	-1.923046	1.827499	H	0.699443	2.21885	1.912381
C	1.180175	-1.883638	-1.46356	C	-1.220714	1.916706	-1.466466
H	1.734385	-1.88641	-2.392371	H	-1.729948	1.848235	-2.419026
C	0.727061	-1.032194	0.768403	C	-0.874471	1.227391	0.838491
C	1.280911	-0.013583	1.621071	C	-1.447635	0.242733	1.721963
C	-3.761971	-0.928653	1.148796	C	4.236644	0.805951	1.092933
C	-3.374351	-3.11273	-0.02243	C	3.845215	2.951417	-0.102782
C	-3.54419	-0.904206	-1.228114	C	3.944179	0.755553	-1.292811
C	-3.685747	0.4703	-1.231519	C	3.961912	-0.625517	-1.26985
C	3.096271	1.607978	1.45361	C	-3.186285	-1.464985	1.553747
H	3.918426	2.05791	0.917776	H	-3.961714	-1.97671	1.002855
C	0.949233	0.457132	2.887856	C	-1.175142	-0.139741	3.031264
H	0.125699	0.01959	3.438007	H	-0.404832	0.367632	3.59844
C	2.745571	2.059655	2.714064	C	-2.889126	-1.831026	2.857226
H	3.310312	2.871519	3.154192	H	-3.448318	-2.638028	3.313973
C	-3.912032	0.443579	1.155088	C	4.250684	-0.57356	1.128177
C	1.687727	1.492978	3.430712	C	-1.899091	-1.176977	3.595283
H	1.44919	1.865948	4.418223	H	-1.70192	-1.480423	4.615197

CB-An at S_1

B	-2.72116	-3.812224	1.398916	B	2.906009	3.631253	1.159779
H	-2.439838	-3.114793	2.305162	H	2.668142	2.937421	2.095405
B	-4.390124	-4.103904	0.907988	B	4.668745	4.009135	0.812535
H	-5.250951	-3.563751	1.51428	H	5.547793	3.571456	1.483726
B	-1.770675	-5.227697	-0.860642	B	1.900708	5.195315	-0.890438
H	-0.79658	-5.493068	-1.477065	H	0.993603	5.555899	-1.568466
B	-4.428616	-4.158828	-0.853971	B	4.650626	4.065745	-0.974068
H	-5.312022	-3.650623	-1.455257	H	5.512545	3.668876	-1.690475
B	-1.732228	-5.178451	0.897296	B	1.922226	5.146751	0.895867
H	-0.72948	-5.384188	1.490218	H	1.029381	5.450998	1.617349
B	-3.380698	-5.437214	1.487296	B	3.605411	5.286251	1.40243
H	-3.578892	-5.933287	2.545681	H	3.837476	5.766376	2.464433
B	-2.779441	-3.892594	-1.418573	B	2.883248	3.703407	-1.291941
H	-2.494117	-3.243793	-2.360459	H	2.575141	3.070541	-2.250579
B	-4.437535	-5.665265	0.077038	B	4.638682	5.568081	-0.027555
H	-5.410776	-6.341424	0.11854	H	5.595133	6.273814	-0.014553
B	-3.435129	-5.521793	-1.383007	B	3.568662	5.372119	-1.445928
H	-3.662619	-6.086563	-2.400376	H	3.759341	5.925666	-2.480145
B	-2.795484	-6.326919	0.067515	B	3.015246	6.238448	0.014161
H	-2.56118	-7.489081	0.093456	H	2.8348	7.412875	0.048006
H	-3.826748	-1.464136	2.085603	H	4.346814	1.366358	2.010364
H	-4.073928	0.963917	2.089055	H	4.369418	-1.100901	2.066277
H	-3.653462	1.010491	-2.16758	H	3.845339	-1.192913	-2.184543
H	-3.40891	-1.413636	-2.170683	H	3.820347	1.274055	-2.232384
N	2.486053	-0.077838	-0.307672	N	-2.548169	0.146049	-0.264622
C	-3.855007	1.171286	-0.03599	C	4.085013	-1.287547	-0.053304
N	-3.963387	2.564794	-0.022467	N	3.969148	-2.71476	-0.003943
C	-3.379771	3.306459	1.028911	C	2.884137	-3.251642	0.665431
C	-4.071255	4.372739	1.601482	C	2.968826	-4.513207	1.288618
C	-2.105172	2.988233	1.496661	C	1.696573	-2.501381	0.777759
C	-3.49054	5.110502	2.620507	C	1.882482	-5.011966	1.973815
H	-5.061091	4.618015	1.239654	H	3.902168	-5.058002	1.270441
C	-1.539699	3.719936	2.528675	C	0.618188	-3.019826	1.461207
H	-1.559972	2.166208	1.051223	H	1.633574	-1.528289	0.313001
C	-2.226007	4.786607	3.092923	C	0.702894	-4.27549	2.058926
H	-4.038056	5.936676	3.056144	H	1.960993	-5.970011	2.469723
H	-0.549144	3.456465	2.877691	H	-0.293582	-2.442888	1.537723
H	-1.779157	5.361572	3.893419	H	-0.144192	-4.667573	2.60489
C	-4.598071	3.24545	-1.082089	C	4.927118	-3.484505	-0.641753
C	-4.041193	4.411512	-1.605883	C	4.601489	-4.732699	-1.203425
C	-5.796339	2.765963	-1.610997	C	6.233879	-2.984354	-0.77748
C	-4.677366	5.084761	-2.636297	C	5.57258	-5.468864	-1.84922
H	-3.111657	4.785039	-1.197289	H	3.580724	-5.086046	-1.166075
C	-6.414752	3.435615	-2.654182	C	7.192499	-3.738556	-1.419546
H	-6.236916	1.867539	-1.19913	H	6.475936	-2.018902	-0.357582
C	-5.86306	4.599997	-3.170555	C	6.872378	-4.983263	-1.954886
H	-4.233688	5.989546	-3.032046	H	5.310719	-6.418653	-2.295449
H	-7.343903	3.050609	-3.054739	H	8.20013	-3.355281	-1.503962

H	-6.353294	5.125063	-3.979665	H	7.627936	-5.564251	-2.465824
C	3.412201	0.263566	-1.367518	C	-3.42767	-0.261409	-1.337605
C	4.835013	-2.129267	-0.494396	C	-4.908547	2.144588	-0.617992
C	5.511654	-0.876827	-0.577912	C	-5.567098	0.880654	-0.667084
C	5.48715	-3.262274	-0.113724	C	-5.586545	3.283345	-0.305925
C	4.870676	0.311939	-0.973496	C	-4.898709	-0.314822	-0.991712
C	6.906299	-0.860293	-0.25184	C	-6.97078	0.858151	-0.382194
C	6.864096	-3.234739	0.217275	C	-6.972495	3.250464	-0.015208
H	4.944899	-4.197422	-0.059222	H	-5.057495	4.226989	-0.275298
C	5.600953	1.511937	-1.064453	C	-5.611145	-1.527178	-1.053198
C	7.613778	0.331197	-0.343779	C	-7.659829	-0.346108	-0.442711
C	7.550536	-2.064149	0.147752	C	-7.642212	2.068847	-0.054435
H	7.361801	-4.146138	0.521644	H	-7.490454	4.167162	0.234748
C	5.03151	2.766095	-1.447505	C	-5.01564	-2.788165	-1.368693
C	7.001248	1.510504	-0.743306	C	-7.020287	-1.532371	-0.773172
H	8.670314	0.340136	-0.101134	H	-8.722918	-0.359679	-0.230701
H	8.604998	-2.024297	0.392489	H	-8.703048	2.024887	0.16034
C	5.779683	3.901031	-1.516096	C	-5.746486	-3.935632	-1.412009
H	3.97916	2.836116	-1.680583	H	-3.956717	-2.850575	-1.572532
C	7.749545	2.718305	-0.833852	C	-7.749572	-2.753591	-0.834281
C	7.162995	3.883417	-1.210831	C	-7.137951	-3.925189	-1.145948
H	5.31045	4.832055	-1.8072	H	-5.257875	-4.87091	-1.654016
H	8.804474	2.683229	-0.590262	H	-8.811586	-2.723266	-0.622703
H	7.740797	4.795938	-1.275504	H	-7.702445	-4.847316	-1.189581
H	3.29226	-0.494046	-2.141751	H	-3.291919	0.46151	-2.141896
H	3.102565	1.202101	-1.823153	H	-3.090531	-1.215239	-1.740398
H	3.782242	-2.19044	-0.72534	H	-3.850038	2.211407	-0.819463

	CB-Bu at S_0				**CB-Bu** at S_1		
C	0.395018	-2.05991	0.550069	C	1.625792	-1.354286	0.613612
C	-2.322898	-2.357219	0.062745	C	-0.570265	-3.055498	0.33452
C	-3.784969	-2.425786	-0.249638	C	-1.744461	-3.89964	0.10687
C	-1.379107	-2.463711	-0.972249	C	0.412747	-2.936921	-0.67298
H	-1.719103	-2.661389	-1.978066	H	0.29291	-3.520111	-1.575776
C	-3.804417	0.310686	-0.384831	C	-3.886688	-1.4552	-0.460929
C	1.577341	-1.575838	2.393436	C	2.235896	0.12295	2.194721
C	-1.88164	-2.15242	1.363901	C	-0.421905	-2.301843	1.497462
H	-2.587051	-2.094877	2.179599	H	-1.165255	-2.37107	2.278852
C	-0.024817	-2.316659	-0.749638	C	1.507309	-2.10798	-0.551304
H	0.681446	-2.383437	-1.565493	H	2.23772	-2.035423	-1.345569
C	-0.525309	-1.995583	1.61325	C	0.663269	-1.444239	1.632558
C	0.235208	-1.695524	2.800388	C	1.054145	-0.498815	2.650102
C	-3.576826	0.917775	0.849316	C	-4.34133	-0.765625	0.673804
C	-4.608489	-0.943653	-0.498941	C	-3.773035	-2.912838	-0.445284
C	-3.225384	0.892782	-1.510897	C	-3.479906	-0.699433	-1.569939
C	-2.384006	1.983837	-1.40435	C	-3.437197	0.680162	-1.517065
C	2.593081	-1.282379	3.29663	C	2.890467	1.085673	2.956813
H	3.622066	-1.202007	2.973451	H	3.810499	1.53948	2.614363

C	-0.096087	-1.511786	4.139887	C	0.518463	-0.137764	3.882585
H	-1.123484	-1.601693	4.469342	H	-0.383429	-0.614129	4.245989
C	2.236351	-1.102977	4.622421	C	2.333796	1.429532	4.178415
H	3.006179	-0.876337	5.34894	H	2.829871	2.170885	4.79219
C	-2.745064	2.013777	0.964808	C	-4.297795	0.611939	0.739612
C	0.907469	-1.21412	5.043517	C	1.158308	0.82996	4.639627
H	0.665296	-1.068108	6.087757	H	0.754282	1.114854	5.602296
B	-4.894654	-1.854908	0.917115	B	-3.194674	-3.652522	0.98803
H	-4.495549	-1.45761	1.95035	H	-3.155024	-2.981598	1.96872
B	-6.211806	-1.071854	0.047642	B	-4.839267	-3.93824	0.223393
H	-6.68928	-0.099638	0.524372	H	-5.831965	-3.46487	0.676488
B	-4.445523	-3.627236	-1.252565	B	-1.802259	-5.240575	-0.80136
H	-3.69548	-4.440674	-1.672844	H	-0.777286	-5.63791	-1.252876
B	-5.823341	-1.144441	-1.669075	B	-4.398892	-3.97492	-1.50847
H	-6.03476	-0.221738	-2.37954	H	-5.046532	-3.526925	-2.399231
B	-4.834145	-3.556281	0.463964	B	-2.246344	-5.211081	0.929981
H	-4.351222	-4.317676	1.230268	H	-1.565635	-5.567333	1.835477
B	-6.390268	-2.729772	0.64458	B	-4.006323	-5.273338	1.019296
H	-7.104275	-2.972381	1.559431	H	-4.506023	-5.753648	1.984625
B	-4.273525	-1.96889	-1.823778	B	-2.592039	-3.697912	-1.390524
H	-3.449054	-1.638244	-2.596553	H	-2.03679	-3.070392	-2.234321
B	-6.97204	-2.300196	-0.977594	B	-4.681048	-5.486694	-0.621045
H	-8.126192	-2.23487	-1.241843	H	-5.64428	-6.144103	-0.851402
B	-5.755862	-2.846501	-2.152172	B	-3.296617	-5.328289	-1.74027
H	-6.012151	-3.174874	-3.262251	H	-3.260799	-5.860048	-2.802489
B	-6.121712	-3.833209	-0.720714	B	-3.14645	-6.237468	-0.210624
H	-6.653222	-4.890469	-0.797263	H	-3.032738	-7.419687	-0.161792
H	-4.056424	0.533799	1.737564	H	-4.696618	-1.331653	1.523071
H	-2.572023	2.458535	1.935154	H	-4.615193	1.132499	1.634311
H	-1.920742	2.393507	-2.291283	H	-3.075429	1.252411	-2.361929
H	-3.410459	0.473547	-2.489358	H	-3.156586	-1.21124	-2.464604
N	1.662423	-1.81088	1.031285	N	2.576818	-0.406575	0.963117
C	-2.09819	2.538139	-0.155825	C	-3.818185	1.33216	-0.349155
N	-1.177375	3.58398	-0.019635	N	-3.651345	2.7499	-0.238189
C	-0.282171	3.597191	1.071057	C	-2.75006	3.223643	0.69919
C	0.070547	4.805364	1.67181	C	-2.936162	4.478371	1.313023
C	0.264744	2.40973	1.561166	C	-1.663552	2.415663	1.08837
C	0.95771	4.821961	2.735997	C	-2.039595	4.914314	2.264315
H	-0.354634	5.72748	1.298314	H	-3.809073	5.06842	1.071765
C	1.130856	2.433823	2.643769	C	-0.773802	2.871367	2.03721
H	-0.003582	1.466918	1.102617	H	-1.52509	1.44834	0.627765
C	1.488459	3.63949	3.232486	C	-0.953759	4.120493	2.626967
H	1.221008	5.768605	3.190703	H	-2.200142	5.868131	2.748486
H	1.526388	1.50038	3.026219	H	0.062199	2.248928	2.326796
H	2.16859	3.656099	4.073905	H	-0.257972	4.463939	3.380201
C	-1.057585	4.556918	-1.034647	C	-4.375065	3.575525	-1.081686
C	-2.19958	5.143495	-1.578874	C	-3.855935	4.810118	-1.512555
C	0.196949	4.944316	-1.503427	C	-5.626736	3.147185	-1.557186

C	-2.085084	6.091738	-2.582347	C	-4.592081	5.60288	-2.367867
H	-3.173436	4.849316	-1.209895	H	-2.863052	5.108562	-1.207069
C	0.302275	5.907653	-2.49382	C	-6.350844	3.957213	-2.405505
H	1.084358	4.487981	-1.084939	H	-6.015627	2.192469	-1.234176
C	-0.835325	6.483255	-3.042415	C	-5.843605	5.187975	-2.813076
H	-2.980543	6.537727	-2.99607	H	-4.178683	6.54178	-2.710462
H	1.2828	6.199761	-2.847842	H	-7.320994	3.629076	-2.752636
H	-0.748955	7.230398	-3.820254	H	-6.413729	5.813227	-3.486502
C	2.818259	-1.623295	0.236766	C	3.724953	-0.079676	0.212399
C	3.325262	-2.676939	-0.5073	C	4.593645	-1.085601	-0.18747
C	3.420718	-0.37427	0.201639	C	3.980324	1.242512	-0.124305
C	4.446332	-2.491882	-1.312997	C	5.725922	-0.785114	-0.938363
H	2.836498	-3.640337	-0.440099	H	4.373823	-2.103514	0.106495
C	4.552328	-0.160814	-0.578657	C	5.116867	1.579424	-0.853545
H	2.982145	0.428516	0.780677	H	3.271145	2.000353	0.182173
C	5.041611	-1.231362	-1.326815	C	5.96909	0.551315	-1.252585
H	5.914273	-1.077592	-1.941895	H	6.848592	0.797817	-1.826001
C	5.193162	1.224947	-0.600112	C	5.376265	3.043899	-1.201358
C	4.173098	2.246206	-1.116442	C	4.216423	3.577456	-2.048686
H	3.847687	1.995203	-2.127299	H	4.121058	3.012584	-2.977257
H	3.288366	2.293578	-0.480116	H	3.264969	3.512092	-1.519645
H	4.619174	3.242879	-1.139832	H	4.385268	4.626084	-2.303583
C	6.424693	1.280631	-1.499348	C	6.669014	3.234789	-1.989603
H	6.84679	2.286406	-1.476593	H	6.810835	4.294811	-2.206084
H	7.202082	0.590103	-1.167134	H	7.540672	2.893716	-1.428364
H	6.180461	1.050846	-2.538054	H	6.645062	2.705163	-2.943503
C	5.617679	1.608454	0.821475	C	5.479702	3.860756	0.090837
H	6.339693	0.893521	1.219754	H	6.300402	3.501519	0.713868
H	6.082651	2.596523	0.82205	H	5.663287	4.91255	-0.139291
H	4.766687	1.644574	1.502695	H	4.563211	3.805222	0.67978
C	4.98227	-3.664524	-2.131255	C	6.657234	-1.915143	-1.371494
C	6.204806	-3.283354	-2.961292	C	7.841958	-1.409975	-2.190159
H	6.5442	-4.151323	-3.528456	H	8.470946	-2.25369	-2.477833
H	5.979237	-2.49067	-3.67695	H	7.520116	-0.912493	-3.106935
H	7.036044	-2.955816	-2.334348	H	8.463689	-0.716404	-1.621001
C	3.889436	-4.155762	-3.086513	C	5.873402	-2.91454	-2.228759
H	3.001704	-4.492424	-2.549749	H	5.037444	-3.351659	-1.681728
H	3.586623	-3.363541	-3.77327	H	5.474054	-2.432803	-3.122848
H	4.255756	-4.996657	-3.679028	H	6.524221	-3.731995	-2.545854
C	5.380506	-4.802582	-1.185605	C	7.202177	-2.627856	-0.129287
H	6.159941	-4.479828	-0.493614	H	7.766158	-1.937865	0.500423
H	4.534422	-5.154987	-0.594837	H	6.403443	-3.056438	0.476571
H	5.762813	-5.651189	-1.756726	H	7.868093	-3.441709	-0.423688

	CB-Cz at S_0				**CB-Cz** at S_1		
C	0.275314	1.744887	1.312693	C	-0.384729	1.878712	1.24574
C	2.812995	2.758145	0.808586	C	1.923126	3.353921	0.726745
C	4.167698	3.33683	0.538062	C	3.137772	4.110118	0.424938

C	1.935779	2.437364	-0.237579	C	1.003543	3.036431	-0.292911
H	2.246442	2.594154	-1.258902	H	1.209169	3.381259	-1.296892
C	5.110008	0.855842	-0.194478	C	5.284625	1.616135	-0.30062
C	-0.825375	1.233484	3.209156	C	-1.198502	0.900356	3.110533
C	2.402451	2.562852	2.122047	C	1.655304	2.920589	2.025071
H	3.060335	2.813028	2.942403	H	2.348529	3.157545	2.820627
C	0.672883	1.926794	-0.005879	C	-0.143623	2.305153	-0.055669
H	0.022663	1.680812	-0.833662	H	-0.82265	2.072318	-0.864734
C	1.137941	2.054347	2.379786	C	0.509452	2.182831	2.285401
C	0.433124	1.72853	3.594063	C	-0.014938	1.565155	3.479781
C	5.025251	-0.056097	0.855449	C	5.577841	0.811963	0.808643
C	5.420799	2.299349	0.035455	C	5.145784	3.0673	-0.172435
C	4.925194	0.374155	-1.489663	C	5.116523	0.987697	-1.543116
C	4.632773	-0.954327	-1.728628	C	5.207381	-0.384244	-1.669948
C	-1.778319	0.855225	4.147084	C	-1.974308	0.220734	4.041981
H	-2.754036	0.497183	3.849098	H	-2.89724	-0.267728	3.760252
C	0.752278	1.826757	4.944876	C	0.407045	1.531709	4.804436
H	1.717339	2.207083	5.254728	H	1.313199	2.04419	5.101673
C	-1.436747	0.962463	5.48437	C	-1.531328	0.200797	5.354422
H	-2.160017	0.673115	6.235711	H	-2.118255	-0.321168	6.099305
C	4.743349	-1.388646	0.626304	C	5.660854	-0.563117	0.696298
C	-0.185219	1.437986	5.883827	C	-0.352311	0.844561	5.735457
H	0.04758	1.507266	6.938001	H	-0.036271	0.812037	6.769789
B	5.420324	2.914371	1.625477	B	4.604453	3.77896	1.274101
H	5.161345	2.193801	2.520914	H	4.533856	3.088795	2.240932
B	6.908017	2.81669	0.687229	B	6.251585	4.050484	0.502075
H	7.685358	1.969581	0.966555	H	7.237417	3.536792	0.924841
B	4.377039	4.883432	-0.147017	B	3.22954	5.46672	-0.457439
H	3.391534	5.47726	-0.422382	H	2.207487	5.897982	-0.882867
B	6.484148	3.134257	-0.992811	B	5.776486	4.138902	-1.218423
H	6.980453	2.511444	-1.867913	H	6.395361	3.69462	-2.132225
B	4.798247	4.562201	1.532443	B	3.703548	5.374297	1.267801
H	4.106648	4.948889	2.411078	H	3.05064	5.731363	2.193949
B	6.540116	4.267327	1.629606	B	5.464168	5.383165	1.336662
H	7.146045	4.525255	2.615475	H	5.984358	5.831103	2.306853
B	4.746302	3.425386	-1.063275	B	3.959107	3.901287	-1.073416
H	4.077622	3.019594	-1.943936	H	3.396711	3.294627	-1.92895
B	7.203348	4.417319	-0.011139	B	6.118453	5.62078	-0.309956
H	8.31041	4.786845	-0.22057	H	7.096356	6.254229	-0.546233
B	5.856885	4.784727	-1.111585	B	4.71139	5.525046	-1.408878
H	5.976483	5.409958	-2.111678	H	4.681505	6.076769	-2.461121
B	5.901842	5.496107	0.514985	B	4.615734	6.404008	0.142588
H	6.053281	6.657505	0.699761	H	4.53703	7.587163	0.226391
H	5.197759	0.2686	1.87066	H	5.72605	1.280076	1.77111
H	4.69096	-2.07555	1.459586	H	5.873978	-1.175533	1.563374
H	4.479595	-1.295892	-2.742932	H	5.064559	-0.860005	-2.632025
H	5.003589	1.04876	-2.330678	H	4.906411	1.594236	-2.412527
N	-0.909785	1.245986	1.820975	N	-1.418749	1.097571	1.752983

C	4.525931	-1.859851	-0.670407	C	5.468115	-1.157242	-0.544318
N	4.213751	-3.202536	-0.902249	N	5.522946	-2.587015	-0.664215
C	3.440282	-3.92982	0.026426	C	4.517978	-3.333834	-0.076709
C	3.768818	-5.250693	0.329241	C	4.760068	-4.642328	0.386143
C	2.333032	-3.345505	0.642207	C	3.24604	-2.758678	0.106199
C	2.998674	-5.97257	1.226684	C	3.740266	-5.363599	0.968827
H	4.628319	-5.704959	-0.145524	H	5.756812	-5.05585	0.324819
C	1.581917	-4.068554	1.555031	C	2.237745	-3.500034	0.682184
H	2.070912	-2.322357	0.406393	H	3.068229	-1.747593	-0.229203
C	1.904656	-5.387042	1.848532	C	2.472284	-4.805369	1.108738
H	3.266713	-6.997177	1.450992	H	3.937606	-6.360632	1.338417
H	0.726297	-3.603149	2.027813	H	1.254539	-3.065826	0.798695
H	1.309771	-5.949581	2.555875	H	1.671836	-5.375633	1.559829
C	4.648732	-3.840821	-2.085198	C	6.563634	-3.147441	-1.380757
C	5.963628	-3.692809	-2.523892	C	7.79197	-2.464855	-1.460736
C	3.768492	-4.63294	-2.820145	C	6.398443	-4.359892	-2.07894
C	6.383181	-4.317981	-3.687091	C	8.832562	-3.011189	-2.179174
H	6.649934	-3.085055	-1.948877	H	7.910335	-1.527119	-0.93819
C	4.201986	-5.269948	-3.971742	C	7.448796	-4.884628	-2.80062
H	2.747621	-4.746491	-2.479996	H	5.433091	-4.845603	-2.086878
C	5.507978	-5.112614	-4.414668	C	8.672239	-4.222037	-2.848731
H	7.406518	-4.193615	-4.017476	H	9.77948	-2.490911	-2.219853
H	3.508438	-5.883047	-4.533002	H	7.308422	-5.804364	-3.351895
H	5.841216	-5.60568	-5.318298	H	9.491008	-4.63792	-3.41966
C	-2.027304	0.849688	1.063822	C	-2.472641	0.547199	1.011515
C	-2.570447	1.722291	0.128256	C	-3.272152	1.362377	0.217316
C	-2.583508	-0.408771	1.261228	C	-2.71286	-0.822045	1.068868
C	-3.678898	1.330304	-0.614975	C	-4.320258	0.806773	-0.509581
H	-2.135533	2.700706	-0.020719	H	-3.080789	2.425305	0.168656
C	-3.694526	-0.792363	0.517507	C	-3.755469	-1.369825	0.333658
H	-2.160089	-1.083354	1.992101	H	-2.090052	-1.457314	1.683068
C	-4.242863	0.073869	-0.421827	C	-4.56689	-0.561848	-0.452679
H	-5.106743	-0.227345	-0.997603	H	-5.383953	-0.992911	-1.014282
C	-3.601957	-3.271989	0.684316	C	-3.061685	-3.73731	0.063143
C	-5.611051	-2.295872	1.001094	C	-5.154697	-3.373959	0.805956
C	-2.26616	-3.538502	0.406447	C	-1.773041	-3.599805	-0.440886
C	-4.521557	-4.30525	0.940807	C	-3.641676	-5.002708	0.276096
C	-6.653211	-1.392451	1.17332	C	-6.339751	-2.799732	1.250295
C	-5.804464	-3.681432	1.145525	C	-4.981298	-4.769197	0.753317
C	-1.860739	-4.862906	0.410119	C	-1.064477	-4.758273	-0.71376
H	-1.56527	-2.745488	0.183124	H	-1.348298	-2.623096	-0.631606
C	-4.089104	-5.627856	0.939332	C	-2.904964	-6.150397	-0.000458
C	-7.903821	-1.905838	1.47187	C	-7.360688	-3.654119	1.62816
H	-6.497845	-0.326023	1.08474	H	-6.460694	-1.726304	1.30214
C	-7.071608	-4.171805	1.446061	C	-6.024679	-5.606018	1.139295
C	-2.758552	-5.89924	0.678154	C	-1.617603	-6.022387	-0.490709
H	-0.824171	-5.094565	0.202013	H	-0.064415	-4.680018	-1.121423
H	-4.787244	-6.431879	1.135296	H	-3.338151	-7.129997	0.15767

C	-8.116847	-3.280204	1.603377	C	-7.210706	-5.042781	1.572216
H	-8.732805	-1.2234	1.608003	H	-8.295686	-3.234324	1.976014
H	-7.234145	-5.236234	1.558953	H	-5.90724	-6.681745	1.10306
H	-2.407753	-6.922766	0.674365	H	-1.037959	-6.907488	-0.718201
H	-9.107997	-3.646855	1.835113	H	-8.031362	-5.680021	1.873737
C	-4.605954	3.523471	-1.325412	C	-5.781393	2.783847	-0.874464
C	-4.487835	1.904909	-2.89308	C	-5.437009	1.424164	-2.641508
C	-4.5731	4.253189	-0.142938	C	-5.80888	3.36582	0.38741
C	-5.110647	4.073269	-2.517514	C	-6.506205	3.324409	-1.951606
C	-4.243943	0.731043	-3.596183	C	-4.994524	0.42849	-3.504527
C	-5.033209	3.040036	-3.519446	C	-6.284611	2.457123	-3.0811
C	-5.034757	5.557905	-0.181524	C	-6.559949	4.517943	0.545728
H	-4.20824	3.821103	0.778705	H	-5.269042	2.937285	1.220488
C	-5.569075	5.387018	-2.52946	C	-7.253862	4.483236	-1.766023
C	-4.579291	0.706638	-4.939276	C	-5.436647	0.472601	-4.815847
H	-3.802141	-0.132907	-3.119042	H	-4.32235	-0.350233	-3.171364
C	-5.361232	2.989484	-4.870734	C	-6.714217	2.478849	-4.404288
C	-5.523998	6.124809	-1.360716	C	-7.272902	5.077132	-0.517479
H	-5.016779	6.148452	0.725326	H	-6.593333	4.993411	1.517424
H	-5.958933	5.822496	-3.440772	H	-7.814272	4.91069	-2.587827
C	-5.136439	1.819702	-5.573229	C	-6.291196	1.482208	-5.264712
H	-4.401802	-0.196637	-5.508554	H	-5.107661	-0.29247	-5.507255
H	-5.781953	3.856176	-5.364661	H	-7.366131	3.268885	-4.754975
H	-5.874471	7.148335	-1.355423	H	-7.846321	5.980727	-0.358832
H	-5.388219	1.765049	-6.624001	H	-6.618083	1.485769	-6.296065
N	-4.230579	2.206696	-1.561514	N	-5.135594	1.629742	-1.301369
N	-4.271483	-2.055741	0.7216	N	-3.984664	-2.75862	0.387628

	CB-CF_3 at S_0				**CB-CF_3** at S_1		
C	1.546746	-1.204762	0.637347	C	1.64257	-1.395591	0.639763
C	-0.638243	-2.888698	0.313839	C	-0.583042	-3.060057	0.380006
C	-1.79439	-3.814721	0.0893	C	-1.770846	-3.88681	0.164371
C	0.422636	-2.884146	-0.60526	C	0.398001	-2.965811	-0.63063
H	0.385962	-3.549651	-1.455579	H	0.266634	-3.553597	-1.52868
C	-3.420644	-1.643155	-0.373045	C	-3.881256	-1.422318	-0.455655
C	2.050616	0.38127	2.157255	C	2.271919	0.097088	2.212748
C	-0.597378	-2.025506	1.400326	C	-0.417712	-2.299344	1.536258
H	-1.405474	-2.001097	2.115242	H	-1.1602	-2.348019	2.319972
C	1.519095	-2.057027	-0.459345	C	1.506878	-2.153081	-0.519351
H	2.316251	-2.072913	-1.189435	H	2.228574	-2.100421	-1.323116
C	0.487564	-1.174883	1.559878	C	0.68261	-1.460292	1.660293
C	0.808147	-0.159836	2.53232	C	1.084995	-0.509205	2.669202
C	-3.941751	-0.943587	0.715351	C	-4.38064	-0.715033	0.647936
C	-3.296437	-3.131373	-0.326853	C	-3.783887	-2.88279	-0.415222
C	-3.048933	-0.910389	-1.498093	C	-3.417534	-0.685489	-1.553416
C	-3.146161	0.46769	-1.521567	C	-3.370521	0.695529	-1.5185
C	2.673408	1.37018	2.908638	C	2.939109	1.051909	2.972148
H	3.641314	1.766262	2.633801	H	3.868701	1.492778	2.638965

C	0.164674	0.315765	3.670905	C	0.550957	-0.136133	3.89843
H	-0.791645	-0.092269	3.972237	H	-0.355985	-0.60185	4.262603
C	2.014322	1.826102	4.03757	C	2.384604	1.408645	4.191541
H	2.477804	2.595193	4.64159	H	2.890497	2.145143	4.802669
C	-4.050153	0.432446	0.69882	C	-4.336004	0.664203	0.69518
C	0.771814	1.310877	4.41636	C	1.20089	0.827376	4.651952
H	0.287885	1.685967	5.308506	H	0.798751	1.1216	5.61247
B	-3.075374	-3.854754	1.211465	B	-3.22045	-3.598088	1.035166
H	-3.028912	-3.166794	2.1663	H	-3.173651	-2.903123	1.999004
B	-4.555958	-4.092277	0.283179	B	-4.866873	-3.878133	0.271414
H	-5.532615	-3.526724	0.638674	H	-5.854486	-3.382278	0.711103
B	-1.590367	-5.29507	-0.721956	B	-1.84617	-5.245244	-0.715424
H	-0.493817	-5.589427	-1.053632	H	-0.825288	-5.664848	-1.155749
B	-4.117126	-4.142258	-1.424012	B	-4.42283	-3.957727	-1.457418
H	-4.788912	-3.604698	-2.236158	H	-5.060198	-3.519962	-2.360229
B	-2.027703	-5.250057	0.981761	B	-2.294722	-5.171588	1.014412
H	-1.228733	-5.487087	1.821298	H	-1.621689	-5.516756	1.929867
B	-3.781623	-5.457899	1.100777	B	-4.055355	-5.206989	1.099254
H	-4.273746	-5.949308	2.060766	H	-4.564313	-5.658815	2.073276
B	-2.369782	-3.927672	-1.519098	B	-2.612104	-3.703416	-1.338508
H	-1.818702	-3.28679	-2.340754	H	-2.044774	-3.104939	-2.19529
B	-4.422746	-5.649669	-0.545433	B	-4.728346	-5.446551	-0.538353
H	-5.390636	-6.294544	-0.775808	H	-5.700148	-6.094835	-0.757285
B	-3.058927	-5.535525	-1.678232	B	-3.338753	-5.331446	-1.656127
H	-3.01884	-6.090948	-2.724755	H	-3.306915	-5.885689	-2.706656
B	-2.860076	-6.362921	-0.116731	B	-3.20603	-6.209713	-0.10689
H	-2.675974	-7.531673	-0.040288	H	-3.108818	-7.391835	-0.032113
H	-4.288445	-1.483015	1.585763	H	-4.774246	-1.267123	1.489553
H	-4.46136	0.950762	1.554087	H	-4.690431	1.198757	1.567462
H	-2.831392	1.012266	-2.400958	H	-2.968675	1.253874	-2.354503
H	-2.662043	-1.416889	-2.369902	H	-3.056883	-1.210986	-2.425492
N	2.49154	-0.261841	1.005511	N	2.608657	-0.451097	0.982137
C	-3.633998	1.16629	-0.415127	C	-3.805298	1.364567	-0.381158
N	-3.70689	2.56123	-0.414532	N	-3.642083	2.787071	-0.287357
C	-3.451578	3.281821	0.773399	C	-2.747547	3.274244	0.648403
C	-4.263227	4.358243	1.127207	C	-2.930725	4.5429	1.234718
C	-2.380194	2.934396	1.595631	C	-1.672426	2.465772	1.068342
C	-4.000678	5.076368	2.282738	C	-2.040161	4.993097	2.184785
H	-5.094866	4.626883	0.489231	H	-3.798076	5.133133	0.974974
C	-2.135927	3.647084	2.758561	C	-0.789208	2.935682	2.015789
H	-1.741143	2.105377	1.320364	H	-1.538762	1.48684	0.632001
C	-2.94079	4.723215	3.106732	C	-0.963869	4.199728	2.575154
H	-4.6384	5.910698	2.545773	H	-2.198378	5.958133	2.64677
H	-1.298385	3.363127	3.383313	H	0.037791	2.31253	2.328791
H	-2.743096	5.283351	4.011233	H	-0.272914	4.555574	3.326991
C	-3.9782	3.267313	-1.605938	C	-4.36441	3.597367	-1.144876
C	-3.251167	4.412726	-1.926652	C	-3.850263	4.831202	-1.586577
C	-4.984164	2.834015	-2.469093	C	-5.608835	3.153378	-1.627145

C	-3.532031	5.11208	-3.089333	C	-4.585174	5.608593	-2.456326
H	-2.470248	4.749826	-1.257995	H	-2.860477	5.138834	-1.280342
C	-5.244553	3.52904	-3.638914	C	-6.332413	3.949229	-2.488381
H	-5.557608	1.951773	-2.216512	H	-5.992424	2.198491	-1.298774
C	-4.524559	4.673091	-3.954454	C	-5.830858	5.179709	-2.905244
H	-2.960115	6.000433	-3.325375	H	-4.175205	6.545507	-2.808086
H	-6.027686	3.180448	-4.300057	H	-7.297161	3.610278	-2.839893
H	-4.736309	5.21808	-4.864838	H	-6.400198	5.793033	-3.590125
C	3.689022	0.005431	0.324612	C	3.740167	-0.129643	0.224799
C	4.570726	-1.029231	0.03186	C	4.568814	-1.137976	-0.260853
C	3.997217	1.30557	-0.060536	C	4.044661	1.19903	-0.052006
C	5.743254	-0.759317	-0.656127	C	5.679583	-0.810711	-1.020882
H	4.345156	-2.036355	0.354723	H	4.349626	-2.170993	-0.028786
C	5.188377	1.56299	-0.720496	C	5.176496	1.510722	-0.789029
H	3.300264	2.106732	0.143501	H	3.387663	1.983998	0.295437
C	6.065622	0.535622	-1.030355	C	5.999187	0.512745	-1.284965
H	6.986932	0.740999	-1.555569	H	6.874611	0.760461	-1.867021
C	5.541815	2.979398	-1.066299	C	5.520617	2.952164	-1.013977
C	6.650986	-1.894423	-1.028895	C	6.526295	-1.908226	-1.595511
F	6.131834	3.592234	-0.037673	F	6.152729	3.469728	0.042503
F	4.45794	3.690258	-1.377484	F	4.425206	3.690361	-1.210119
F	6.380932	3.038981	-2.098499	F	6.314399	3.114505	-2.070375
F	7.907628	-1.485058	-1.192305	F	7.783281	-1.507787	-1.785779
F	6.264836	-2.46173	-2.173512	F	6.055345	-2.309848	-2.777669
F	6.647724	-2.847022	-0.096952	F	6.552953	-2.974568	-0.797842

CB-TPE at S_0

C	-0.37509	-0.970471	1.524166	C	0.335461	1.206149	1.665343
C	-2.538136	-2.641977	1.03017	C	2.551028	2.813771	1.12183
C	-3.673358	-3.568119	0.719789	C	3.71175	3.620586	0.742127
C	-1.306034	-2.829457	0.381844	C	1.346619	2.934484	0.393729
H	-1.200824	-3.641317	-0.323407	H	1.30003	3.667733	-0.399748
C	-5.018796	-1.488289	-0.482443	C	5.393058	1.212171	-0.762703
C	-0.105912	0.851562	2.809239	C	-0.010181	-0.512	3.075702
C	-2.67815	-1.594709	1.930942	C	2.616303	1.868198	2.143811
H	-3.616629	-1.423844	2.436046	H	3.529883	1.753446	2.70961
C	-0.21849	-2.012687	0.617532	C	0.23937	2.15469	0.650503
H	0.718006	-2.177527	0.102796	H	-0.664432	2.268481	0.06732
C	-1.603519	-0.750206	2.173029	C	1.518692	1.057516	2.406802
C	-1.43244	0.41968	2.997047	C	1.297954	-0.041609	3.315707
C	-5.715655	-0.583796	0.318473	C	6.040777	0.29809	0.082534
C	-5.003135	-2.943404	-0.143526	C	5.433575	2.645302	-0.474044
C	-4.36578	-0.990466	-1.607729	C	4.652982	0.701521	-1.838722
C	-4.364725	0.360555	-1.897819	C	4.486358	-0.659062	-2.009113
C	0.405799	1.953257	3.484968	C	-0.547735	-1.568984	3.803171
H	1.431578	2.267322	3.349781	H	-1.560144	-1.908843	3.632581
C	-2.267611	1.116942	3.865402	C	2.078438	-0.650791	4.293242
H	-3.289779	0.795788	4.0211	H	3.080751	-0.292943	4.492372

C	-0.443748	2.6286	4.343635	C	0.252294	-2.160764	4.767824
H	-0.070527	3.489046	4.883985	H	-0.14723	-2.980461	5.351615
C	-5.727222	0.766657	0.032612	C	5.877212	-1.06298	-0.075388
C	-1.767881	2.22101	4.533142	C	1.553444	-1.712478	5.011957
H	-2.402433	2.768593	5.217696	H	2.149114	-2.190569	5.778577
B	-5.169789	-3.367843	1.508499	B	5.301853	3.133973	1.162854
H	-5.291432	-2.513885	2.310262	H	5.436296	2.294595	1.994015
B	-6.424087	-3.743256	0.326354	B	6.728675	3.467515	0.056969
H	-7.416861	-3.099467	0.344306	H	7.74936	2.864168	0.151644
B	-3.393703	-5.178956	0.252956	B	3.679758	5.10237	0.086616
H	-2.272767	-5.556091	0.236362	H	2.620436	5.632082	-0.011112
B	-5.626747	-4.124149	-1.199324	B	5.883587	3.851694	-1.470293
H	-6.068406	-3.734896	-2.225787	H	6.244578	3.543482	-2.560391
B	-4.19025	-4.804816	1.776312	B	4.529352	4.725114	1.613765
H	-3.612467	-4.898376	2.804264	H	4.130915	4.942332	2.711136
B	-5.936983	-4.947176	1.528525	B	6.254624	4.673598	1.252837
H	-6.658366	-5.23793	2.423317	H	7.021146	4.93691	2.121931
B	-3.890788	-3.969454	-0.931097	B	4.142154	3.656211	-0.935796
H	-3.134635	-3.507909	-1.708601	H	3.337205	3.22903	-1.699819
B	-6.21314	-5.43147	-0.158715	B	6.524819	5.153116	-0.446801
H	-7.146384	-6.086806	-0.483915	H	7.46317	5.788462	-0.805749
B	-4.629534	-5.562758	-0.953393	B	4.89949	5.282502	-1.178977
H	-4.396935	-6.306432	-1.847078	H	4.657736	6.004597	-2.091417
B	-4.831283	-6.085592	0.734007	B	5.220778	5.896317	0.46681
H	-4.744071	-7.22313	1.057385	H	5.241639	7.052868	0.740409
H	-6.27535	-0.940811	1.171645	H	6.648441	0.674194	0.893197
H	-6.276739	1.447587	0.667943	H	6.350826	-1.758866	0.605504
H	-3.831327	0.722252	-2.765975	H	3.872713	-1.041881	-2.814735
H	-3.832885	-1.661731	-2.264695	H	4.173232	1.389175	-2.519798
N	0.525183	-0.000829	1.916238	N	-0.587873	0.255821	2.080058
C	-5.032533	1.26635	-1.071582	C	5.075167	-1.538776	-1.107104
N	-5.00948	2.639244	-1.333407	N	4.798644	-2.940741	-1.195929
C	-4.947782	3.558818	-0.262638	C	4.116281	-3.533323	-0.147614
C	-5.735962	4.708291	-0.280671	C	4.322495	-4.889283	0.175599
C	-4.092233	3.333279	0.815209	C	3.247183	-2.756409	0.643342
C	-5.661577	5.618276	0.761592	C	3.651443	-5.448356	1.241427
H	-6.400904	4.881796	-1.116502	H	5.044159	-5.468992	-0.382514
C	-4.03771	4.239765	1.86187	C	2.580012	-3.334753	1.701678
H	-3.471835	2.446537	0.830753	H	3.095992	-1.713694	0.404696
C	-4.817556	5.388025	1.839444	C	2.774757	-4.680423	2.004544
H	-6.278616	6.507465	0.735114	H	3.830729	-6.483582	1.498575
H	-3.366646	4.046799	2.689436	H	1.908305	-2.734703	2.300749
H	-4.767414	6.098452	2.654201	H	2.256652	-5.12221	2.844679
C	-4.981561	3.117492	-2.659789	C	5.199405	-3.630819	-2.327447
C	-4.139059	4.171209	-3.011985	C	4.464331	-4.730679	-2.806255
C	-5.804847	2.549723	-3.632083	C	6.329394	-3.19118	-3.038707
C	-4.12748	4.648265	-4.312734	C	4.876881	-5.387712	-3.94646
H	-3.499085	4.612574	-2.259581	H	3.554313	-5.02557	-2.303121

C	-5.771894	3.021006	-4.934367	C	6.730239	-3.865647	-4.172167
H	-6.468002	1.739314	-3.35937	H	6.883315	-2.338047	-2.674791
C	-4.937785	4.074526	-5.282503	C	6.012891	-4.966945	-4.631289
H	-3.468831	5.467725	-4.57111	H	4.296243	-6.220445	-4.319595
H	-6.416134	2.56956	-5.678114	H	7.611064	-3.532697	-4.703841
H	-4.920986	4.445564	-6.298738	H	6.328617	-5.484687	-5.526693
C	1.858725	0.103545	1.470681	C	-1.895312	0.118976	1.578101
C	2.728193	-0.971951	1.620395	C	-2.747666	1.21811	1.556234
C	2.31158	1.277827	0.878879	C	-2.340924	-1.107562	1.097186
C	4.026219	-0.882482	1.151164	C	-4.019684	1.096498	1.026863
H	2.383018	-1.871101	2.11377	H	-2.410238	2.161861	1.964293
C	3.621509	1.368903	0.440845	C	-3.62657	-1.227044	0.598267
H	1.630697	2.109732	0.754649	H	-1.672832	-1.958839	1.106218
C	4.494075	0.283179	0.541758	C	-4.479116	-0.123236	0.526662
H	4.694568	-1.725351	1.263865	H	-4.67439	1.95716	1.005878
H	3.971448	2.28899	-0.009474	H	-3.971576	-2.186634	0.235003
C	5.890595	0.391768	0.052773	C	-5.848797	-0.264527	-0.025767
C	6.469898	-0.573012	-0.704156	C	-6.364251	0.617183	-0.918082
C	6.5941	1.637484	0.449276	C	-6.60037	-1.445954	0.467499
C	7.283935	2.407977	-0.488264	C	-7.254663	-2.30684	-0.415275
C	6.532398	2.092978	1.768141	C	-6.621141	-1.749809	1.830557
C	7.91003	3.586047	-0.114042	C	-7.926244	-3.424815	0.052695
H	7.32674	2.074273	-1.51669	H	-7.233642	-2.091324	-1.475445
C	7.168596	3.265202	2.145017	C	-7.302823	-2.861516	2.299927
H	5.984218	1.515505	2.502288	H	-6.101378	-1.101509	2.525181
C	7.859894	4.016455	1.204684	C	-7.957998	-3.703582	1.412137
H	8.436753	4.171797	-0.856638	H	-8.424306	-4.082635	-0.648159
H	7.120987	3.59483	3.175205	H	-7.319054	-3.072859	3.361661
H	8.351165	4.935849	1.496532	H	-8.484751	-4.576059	1.776999
C	5.694282	-1.689421	-1.302253	C	-5.532505	1.646146	-1.592697
C	4.521126	-1.45184	-2.020584	C	-4.327286	1.31011	-2.211784
C	6.154585	-3.003693	-1.19638	C	-5.968723	2.971048	-1.661584
C	3.815981	-2.498637	-2.593154	C	-3.568828	2.273928	-2.857266
H	4.16549	-0.435512	-2.129131	H	-3.988813	0.28254	-2.184995
C	5.442588	-4.052028	-1.757525	C	-5.204017	3.937581	-2.295514
H	7.077165	-3.199211	-0.664152	H	-6.914534	3.240227	-1.208117
C	4.269721	-3.803548	-2.4573	C	-4.000345	3.592829	-2.894984
H	2.91247	-2.2934	-3.15344	H	-2.64073	1.992211	-3.33856
H	5.807817	-5.065787	-1.65287	H	-5.55191	4.962309	-2.326423
H	3.71797	-4.621334	-2.902941	H	-3.407036	4.345964	-3.39755
C	7.924013	-0.595669	-1.00028	C	-7.799092	0.629062	-1.297217
C	8.872044	-0.420028	0.009257	C	-8.804684	0.584076	-0.329985
C	8.373365	-0.849586	-2.298107	C	-8.170907	0.741175	-2.638832
C	10.227085	-0.475068	-0.274372	C	-10.140593	0.627978	-0.69472
H	8.537791	-0.240239	1.022518	H	-8.530529	0.515139	0.714445
C	9.728731	-0.891528	-2.584093	C	-9.5073	0.771804	-3.004452
H	7.648814	-1.011582	-3.086362	H	-7.400835	0.80124	-3.397741
C	10.660872	-0.704432	-1.572846	C	-10.497377	0.71538	-2.033331

H	10.946998	-0.341769	0.523091	H	-10.905904	0.597393	0.070363
H	10.057713	-1.076982	-3.598736	H	-9.775992	0.846127	-4.050589
H	11.719784	-0.745393	-1.793932	H	-11.541414	0.747713	-2.317573

Table S3. Coordinates of the optimized S_1 structure of **CB-CF_3** in the ONIOM model

N	4.382002	-2.549639	-0.037041
N	-3.369589	0.9791	0.983044
C	1.174016	3.950731	-0.470938
C	3.337028	2.972934	-0.68913
C	3.621668	1.53609	-0.55205
C	2.822834	0.565926	-1.203739
H	1.970469	0.888011	-1.789796
C	3.118061	-0.776692	-1.107053
H	2.501434	-1.522251	-1.602131
C	4.170141	-1.18426	-0.258812
C	4.961609	-0.245909	0.430634
H	5.792296	-0.581439	1.04841
C	4.707059	1.093261	0.244767
H	5.336852	1.821753	0.737209
C	4.529415	-3.003925	1.262547
C	3.848826	-2.332348	2.30897
H	3.171261	-1.519871	2.07221
C	4.007247	-2.773391	3.604437
H	3.481023	-2.27655	4.411264
C	4.851682	-3.856527	3.881312
H	4.994475	-4.179216	4.907184
C	5.526188	-4.518911	2.847369
H	6.2141	-5.324645	3.075311
C	5.36238	-4.113905	1.538271
H	5.913015	-4.580659	0.729043
C	4.403911	-3.413876	-1.140296
C	3.727459	-4.646554	-1.081038
H	3.181494	-4.929494	-0.185375
C	3.697319	-5.442936	-2.213765
H	3.134972	-6.370221	-2.193006
C	4.378427	-5.04972	-3.373024
H	4.372753	-5.694851	-4.247129
C	5.07462	-3.836051	-3.415553
H	5.628029	-3.553342	-4.306614
C	5.072466	-2.999282	-2.311078
H	5.632679	-2.070012	-2.30446
C	-0.017633	3.175403	-0.155841
C	-0.489193	3.114086	1.163984
H	0.035966	3.65271	1.947977
C	-1.626814	2.373015	1.453015
C	-2.293459	1.668186	0.427129
C	-1.836272	1.704356	-0.893123

H	-2.335016	1.160068	-1.688743
C	-0.713163	2.465715	-1.166363
H	-0.355374	2.53122	-2.188708
C	-2.349557	2.110374	2.681071
C	-2.191199	2.547107	3.997675
H	-1.367869	3.20619	4.263145
C	-3.107856	2.134616	4.956568
H	-3.009104	2.478721	5.981785
C	-4.175136	1.288782	4.611512
H	-4.891439	0.998377	5.374035
C	-4.340624	0.826864	3.310849
H	-5.177181	0.185857	3.049233
C	-3.412833	1.244296	2.354972
C	-4.142695	0.021448	0.301731
C	-4.79567	0.363399	-0.884647
H	-4.73337	1.384068	-1.24947
C	-5.530944	-0.600547	-1.567336
C	-5.626012	-1.903737	-1.088306
H	-6.199935	-2.649547	-1.627829
C	-4.958743	-2.232446	0.088671
C	-4.222824	-1.28352	0.790838
H	-3.679937	-1.553287	1.694107
C	-4.910359	-3.662014	0.554851
C	-6.18678	-0.238324	-2.872811
B	2.603368	3.820988	0.569497
H	2.463615	3.248887	1.603548
B	4.31572	4.129804	-0.079129
H	5.30323	3.806603	0.493877
B	3.35745	5.486414	0.469167
H	3.73558	6.103583	1.41176
B	4.154882	5.529399	-1.124757
H	5.092958	6.189513	-1.386394
B	2.584304	6.267666	-0.92799
H	2.488004	7.452981	-0.992006
B	2.885808	5.180395	-2.321027
H	2.944555	5.559102	-3.446523
B	1.316306	5.172418	-1.532457
H	0.325448	5.474039	-2.116032
B	2.188225	3.576369	-1.811221
H	1.777009	2.832187	-2.642247
B	1.606158	5.337454	0.234117
H	0.851784	5.793639	1.033216
B	4.023263	3.91631	-1.823589
H	4.758283	3.390323	-2.597438
F	-5.937181	-4.381472	0.078783
F	-4.928075	-3.750068	1.891264
F	-3.780297	-4.264073	0.140566
F	-5.33618	-0.391396	-3.906896

F	-7.256667	-1.000646	-3.126272
F	-6.584255	1.043758	-2.894347