Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

Exploring the ESIPT dynamical processes of two novel chromophores: symmetrical structure CHC and asymmetric structure CHN

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Table S1. The calculated potential energy barriers (kcal/mol) among these three stable points on both S_0 and S_1 state PESs for CHC.

S_0				S_1			
forward		backward		forward		backward	
a → b or c	5.70	b or c → a	1.85	A → B or C	6.15	B or C → A	7.67
b or c → d	9.60	d → b or c	0.07	B or C → D	7.62	D → B or C	0.64
a → d	13.77	d → a	0.40	A → D	4.71	D → A	4.19

Table S2. The calculated potential energy barriers (kcal/mol) among these three stable points on both S_0 and S_1 state PESs for CHN.

S_0				S_1			
forward		backward		forward		backward	
a → b	5.00	b → a	1.77	A → B	2.67	B → A	2.53
a → c	5.43	c → a	2.16	A → C	3.04	C → A	4.78
b → d	8.70	d → b	0.41	B → D	6.75	D → B	1.34
c → d	9.27	d → c	0.16	C → D	7.24	D → C	0.06
a → d	12.53	d → a	0.57	A → D	7.69	D → A	2.23

Table S3. Cartesian coordinates of structures (CHC, CHC-S, CHC-D and CHC-O) in S_0 and S_1 states.

1. CHC (S_0)				
Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	4.162372	-1.376889	0.010977
7	0	0.53813	0.43221	-0.011224
8	0	-1.755642	-2.738845	-0.025544
6	0	-2.905823	-2.048703	-0.017654
6	0	-1.698114	0.151887	-0.0067
6	0	-2.918518	-0.627402	-0.007738
6	0	2.918519	0.62743	-0.00776
7	0	-0.538136	-0.432191	-0.011255
6	0	1.69811	-0.151858	-0.0067
6	0	-4.111974	-2.773906	-0.019834
6	0	2.905854	2.048727	-0.017678
6	0	-5.321902	-2.10774	-0.011619
6	0	-4.179918	0.013745	0.000735
6	0	4.112018	2.773909	-0.019856
8	0	1.755695	2.738919	-0.025568
6	0	4.179913	-0.013737	0.00073
6	0	5.321937	2.107724	-0.011622
6	0	5.391904	0.694151	-0.000782
6	0	-5.391895	-0.694166	-0.000779
6	0	6.571739	-1.423388	0.019834
6	0	5.324745	-2.144313	0.021215
8	0	5.175	-3.357221	0.030311
6	0	7.953512	0.65395	0.007991
8	0	-4.1624	1.376897	0.010976
6	0	-6.571769	1.42335	0.019822
6	0	-5.32479	2.144299	0.021221
6	0	6.630641	-0.059692	0.009179
6	0	-6.630646	0.059653	0.009166
8	0	-5.175067	3.35721	0.030344
6	0	-7.953504	-0.654013	0.007962
1	0	-0.997461	-2.087619	-0.021977
1	0	-1.766321	1.239249	-0.00211
1	0	1.766328	-1.239219	-0.002184
1	0	-4.06713	-3.857193	-0.027824
1	0	-6.239334	-2.685087	-0.013432
1	0	4.067193	3.857196	-0.027821
1	0	0.997488	2.087761	-0.021936
1	0	6.239377	2.685058	-0.013408
1	0	7.469304	-2.030453	0.027839
1	0	8.779734	-0.059035	0.015952

1	0	8.04874	1.303079	0.885424
1	0	8.05434	1.28975	-0.878512
1	0	-7.469347	2.030396	0.027817
1	0	-8.779738	0.058958	0.01591
1	0	-8.05431	-1.289816	-0.878542
1	0	-8.048733	-1.303143	0.885394

2. CHC-S (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-4.227715	1.38018	0.001019
7	0	-0.548992	-0.321142	-0.001077
8	0	1.817906	2.795779	-0.002338
6	0	2.950819	2.073835	-0.001609
6	0	1.707938	-0.113227	-0.000662
6	0	2.935608	0.653504	-0.000698
6	0	-2.921904	-0.59373	-0.00079
7	0	0.555668	0.483356	-0.000946
6	0	-1.763638	0.20231	-0.000606
6	0	4.170232	2.77479	-0.001835
6	0	-2.82622	-2.053975	-0.001778
6	0	5.367645	2.086065	-0.001084
6	0	4.185279	-0.01216	0.000093
6	0	-4.06845	-2.787933	-0.002022
8	0	-1.698452	-2.639494	-0.002395
6	0	-4.209912	0.021075	0.000018
6	0	-5.275866	-2.146344	-0.001241
6	0	-5.39187	-0.717002	-0.000144
6	0	5.410272	0.67178	-0.000071
6	0	-6.633415	1.365814	0.001918
6	0	-5.41378	2.122122	0.002038
8	0	-5.28801	3.339302	0.002898
6	0	-7.950179	-0.754795	0.000762
8	0	4.140155	-1.3741	0.001064
6	0	6.548444	-1.468755	0.001855
6	0	5.287538	-2.165505	0.00203
6	0	-6.646922	-0.003992	0.000856
6	0	6.634364	-0.106763	0.000841
8	0	5.113118	-3.374515	0.002917
6	0	7.970445	0.581359	0.000705
1	0	1.04139	2.181701	-0.001996
1	0	1.78224	-1.200741	-0.000397
1	0	-1.823765	1.285572	-0.000037
1	0	4.145527	3.858675	-0.002581
1	0	6.29558	2.646388	-0.001264
1	0	-4.009756	-3.871333	-0.00282

1	0	-0.515824	-1.364494	-0.001589
1	0	-6.184923	-2.738365	-0.001455
1	0	-7.551405	1.941449	0.002731
1	0	-8.796182	-0.065217	0.001695
1	0	-8.030596	-1.400786	0.88204
1	0	-8.031332	-1.399275	-0.881556
1	0	7.433693	-2.093646	0.002585
1	0	8.783077	-0.147077	0.001245
1	0	8.080641	1.221333	-0.881655
1	0	8.080309	1.222271	0.88243

3. CHC-D (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-4.243995	1.390115	0.089627
7	0	-0.580278	-0.357039	-0.070759
8	0	1.690279	2.600583	-0.174677
6	0	2.831087	2.026854	-0.127232
6	0	1.769261	-0.216329	-0.024127
6	0	2.934219	0.573526	-0.045505
6	0	-2.934212	-0.573479	-0.045379
7	0	0.580286	0.357074	-0.070834
6	0	-1.769252	0.21639	-0.02419
6	0	4.06164	2.770437	-0.151994
6	0	-2.831038	-2.026813	-0.126813
6	0	5.274081	2.136763	-0.096209
6	0	4.221847	-0.03376	0.011012
6	0	-4.061559	-2.770446	-0.151456
8	0	-1.690193	-2.600476	-0.174213
6	0	-4.22186	0.033769	0.011052
6	0	-5.274023	-2.136804	-0.095766
6	0	-5.398735	-0.712229	-0.011441
6	0	5.398746	0.712197	-0.011639
6	0	-6.65038	1.359186	0.132639
6	0	-5.434292	2.122805	0.155049
8	0	-5.316263	3.338068	0.224236
6	0	-7.956967	-0.765358	0.029906
8	0	4.24394	-1.390088	0.089831
6	0	6.650328	-1.359236	0.132798
6	0	5.434226	-2.122819	0.155348
6	0	-6.658329	-0.007589	0.051893
6	0	6.658313	0.007526	0.051803
8	0	5.316145	-3.338058	0.224818
6	0	7.956975	0.76525	0.029659
1	0	0.623804	1.421118	-0.124818
1	0	1.819793	-1.299291	0.029225

1	0	-1.81978	1.299364	0.028951
1	0	3.99623	3.851457	-0.214467
1	0	6.179124	2.734409	-0.116128
1	0	-3.996108	-3.851473	-0.213753
1	0	-0.623795	-1.421122	-0.124539
1	0	-6.179047	-2.734483	-0.115576
1	0	-7.570643	1.928879	0.183843
1	0	-8.806529	-0.082617	0.086765
1	0	-8.017533	-1.463549	0.872066
1	0	-8.05006	-1.356356	-0.887965
1	0	7.570579	-1.92894	0.184099
1	0	8.806518	0.082489	0.086562
1	0	8.050045	1.356137	-0.888285
1	0	8.017601	1.463539	0.871734

4. CHC-O (S_0)

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-4.207382	-1.377796	-0.000217
7	0	-0.550168	0.28758	0.000095
8	0	1.766314	-2.671838	-0.000184
6	0	2.966129	-2.033936	0.000018
6	0	1.777835	0.196388	0.000096
6	0	2.952187	-0.616716	0.000111
6	0	-2.952196	0.616749	0.000085
7	0	0.550166	-0.287592	-0.000033
6	0	-1.777847	-0.196366	-0.000031
6	0	4.164342	-2.748299	0.000507
6	0	-2.966169	2.033976	0.000234
6	0	5.380872	-2.095043	0.000397
6	0	4.223855	0.011608	-0.00028
6	0	-4.164396	2.748315	0.000413
8	0	-1.766378	2.67193	0.000261
6	0	-4.22385	-0.011596	-0.000011
6	0	-5.380911	2.09503	0.000347
6	0	-5.434565	0.689025	0.00016
6	0	5.434557	-0.689039	0.000367
6	0	-6.607011	-1.427321	-0.00022
6	0	-5.362004	-2.146969	-0.000377
8	0	-5.216087	-3.352851	-0.000597
6	0	-7.988876	0.636822	0.000179
8	0	4.207426	1.37781	-0.000465
6	0	6.607055	1.42728	-0.000169
6	0	5.362065	2.146956	-0.000505
6	0	-6.667038	-0.071103	0.000029
6	0	6.667047	0.071061	0.000123

8	0	5.216178	3.352841	-0.000786
6	0	7.988868	-0.636897	0.00041
1	0	1.902331	-3.628709	0.000102
1	0	1.888579	1.273368	0.000259
1	0	-1.888608	-1.273346	-0.000197
1	0	4.129652	-3.831579	0.000432
1	0	6.293885	-2.672391	0.000743
1	0	-4.129733	3.831595	0.000549
1	0	-1.902434	3.628796	0.000295
1	0	-6.293937	2.672357	0.000481
1	0	-7.502035	-2.033592	-0.000327
1	0	-8.811118	-0.076214	0.000155
1	0	-8.087501	1.27795	-0.878937
1	0	-8.087397	1.277768	0.879439
1	0	7.502093	2.03353	-0.000302
1	0	8.811129	0.076117	0.000243
1	0	8.087368	-1.277673	0.879797
1	0	8.087478	-1.278201	-0.878579

5. CHC (S_1)

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	4.216161	-1.396161	0.001105
7	0	0.527006	0.392148	-0.000725
8	0	-1.72207	-2.673029	-0.002192
6	0	-2.882436	-2.019876	-0.001595
6	0	-1.731213	0.217613	-0.000437
6	0	-2.910315	-0.568415	-0.000668
6	0	2.910311	0.568392	-0.000586
7	0	-0.527002	-0.392175	-0.000735
6	0	1.731216	-0.217643	-0.000348
6	0	-4.072256	-2.76709	-0.001938
6	0	2.882409	2.01985	-0.001523
6	0	-5.299212	-2.130795	-0.001291
6	0	-4.203608	0.030031	0.000026
6	0	4.072216	2.767083	-0.001914
8	0	1.722027	2.672978	-0.002059
6	0	4.203613	-0.030036	0.000088
6	0	5.299182	2.130807	-0.001293
6	0	5.392417	0.708259	-0.000217
6	0	-5.392425	-0.708246	-0.000237
6	0	6.621629	-1.378227	0.001747
6	0	5.391201	-2.13228	0.002058
8	0	5.280708	-3.350001	0.002928
6	0	7.956385	0.730791	0.000356
8	0	-4.216134	1.396156	0.001032

6	0	-6.621603	1.378259	0.001732
6	0	-5.391163	2.132294	0.002011
6	0	6.64889	-0.011447	0.000643
6	0	-6.648885	0.01148	0.000646
8	0	-5.280651	3.350012	0.00285
6	0	-7.956393	-0.730738	0.000399
1	0	-0.976288	-1.985407	-0.001802
1	0	-1.78996	1.302858	0.000047
1	0	1.789966	-1.302888	0.000158
1	0	-4.000035	-3.849109	-0.002703
1	0	-6.205654	-2.724066	-0.001581
1	0	3.999977	3.849101	-0.002685
1	0	0.976262	1.985341	-0.001563
1	0	6.205614	2.724093	-0.001618
1	0	7.534219	-1.962686	0.002451
1	0	8.796979	0.034844	0.001071
1	0	8.041063	1.375205	0.882102
1	0	8.041451	1.373836	-0.882351
1	0	-7.534183	1.962733	0.002448
1	0	-8.796975	-0.034777	0.001125
1	0	-8.041489	-1.373792	-0.882298
1	0	-8.04106	-1.375139	0.882155

6. CHC-S (S_1)

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	4.260296	-1.389459	-0.000108
7	0	0.535165	0.201874	0.000005
8	0	-1.875514	-2.822557	-0.000199
6	0	-3.005375	-2.085059	-0.000119
6	0	-1.731993	0.083178	-0.000056
6	0	-2.956455	-0.655535	-0.000078
6	0	2.934955	0.541454	0.000058
7	0	-0.563441	-0.552967	-0.000061
6	0	1.768641	-0.305012	-0.000015
6	0	-4.23109	-2.765535	-0.000095
6	0	2.839126	2.002888	0.000166
6	0	-5.427467	-2.066136	-0.000049
6	0	-4.209398	0.017251	-0.000037
6	0	4.06913	2.764982	0.000207
8	0	1.714969	2.587705	0.000131
6	0	4.204294	-0.025048	0.00001
6	0	5.306141	2.159415	0.000177
6	0	5.422806	0.749842	0.00007
6	0	-5.442844	-0.64953	-0.000024
6	0	6.674913	-1.312253	-0.000063

6	0	5.458231	-2.089449	-0.00027
8	0	5.38092	-3.306375	-0.000073
6	0	7.978733	0.819574	0.000182
8	0	-4.146958	1.38307	-0.000004
6	0	-6.548746	1.510511	0.000037
6	0	-5.277636	2.187856	0.000047
6	0	6.678926	0.062236	0.000051
6	0	-6.653295	0.148905	0.000011
8	0	-5.089296	3.397776	0.000032
6	0	-8.000612	-0.517991	0.000014
1	0	-1.095872	-2.206986	-0.000257
1	0	-1.772289	1.170931	-0.000002
1	0	1.855293	-1.383085	-0.000088
1	0	-4.218467	-3.850214	-0.000125
1	0	-6.362547	-2.613703	-0.000039
1	0	3.974169	3.845659	0.000268
1	0	0.485877	1.237801	0.000103
1	0	6.202077	2.768113	0.000228
1	0	7.596047	-1.882281	-0.000018
1	0	8.825091	0.131027	0.000163
1	0	8.05785	1.462222	0.883157
1	0	8.05794	1.462387	-0.882665
1	0	-7.425647	2.147276	0.000053
1	0	-8.802439	0.222547	0.000037
1	0	-8.120206	-1.157276	-0.88166
1	0	-8.120186	-1.157309	0.881667

7. CHC-D (S_1)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-4.256428	1.399511	-0.064036
7	0	-0.576114	-0.331766	0.031516
8	0	1.748604	2.616359	0.109312
6	0	2.876782	2.024581	0.084764
6	0	1.785842	-0.247321	0.006027
6	0	2.957462	0.560278	0.028499
6	0	-2.957403	-0.560006	0.02849
7	0	0.576015	0.332024	0.03155
6	0	-1.785971	0.247681	0.006005
6	0	4.113105	2.764465	0.110578
6	0	-2.876399	-2.024283	0.084771
6	0	5.332144	2.134595	0.077599
6	0	4.231445	-0.032676	-0.005933
6	0	-4.112515	-2.764383	0.110586
8	0	-1.747984	-2.615805	0.109318
6	0	-4.231615	0.032728	-0.005939

6	0	-5.331671	-2.134738	0.07761
6	0	-5.433996	-0.713798	0.016329
6	0	5.434126	0.713673	0.01632
6	0	-6.664094	1.366245	-0.087449
6	0	-5.439475	2.124457	-0.108885
8	0	-5.334765	3.341832	-0.161917
6	0	-7.992465	-0.747356	-0.004425
8	0	4.256039	-1.39944	-0.06402
6	0	6.663758	-1.366591	-0.087464
6	0	5.438967	-2.124578	-0.108879
6	0	-6.683934	-0.005024	-0.025885
6	0	6.683899	0.004689	-0.025903
8	0	5.334085	-3.341906	-0.161905
6	0	7.99259	0.746735	-0.004458
1	0	0.602325	1.380895	0.061811
1	0	1.836654	-1.327795	-0.030749
1	0	-1.836806	1.328159	-0.030792
1	0	4.041102	3.846154	0.155364
1	0	6.239699	2.726796	0.097376
1	0	-4.040341	-3.846063	0.155373
1	0	-0.602785	-1.380794	0.061786
1	0	-6.239105	-2.727134	0.09739
1	0	-7.579547	1.944773	-0.122901
1	0	-8.83244	-0.051624	-0.041438
1	0	-8.085799	-1.351526	0.904309
1	0	-8.071117	-1.428501	-0.858498
1	0	7.579077	-1.945327	-0.122927
1	0	8.832401	0.05081	-0.041492
1	0	8.071384	1.42786	-0.858531
1	0	8.086072	1.35086	0.904287

Table S4. Cartesian coordinates of structures (CHN, CHN-S-1, CHN-S-2, CHN-D and CHN-O) in S_0 and S_1 states.

1. CHN (S_0)				
Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-3.622599	1.37134	0.000165
7	0	-0.033561	-0.509774	0.000003
8	0	2.349306	2.559409	-0.000247
6	0	3.478337	1.827832	-0.000183
6	0	2.211504	-0.29678	0.000038
6	0	3.466292	0.416046	-0.000046
6	0	-2.418123	-0.65684	0.000031
7	0	1.064679	0.324138	-0.000107
6	0	-1.18095	0.098292	0.000027
6	0	4.698625	2.549618	-0.000236
6	0	-2.434371	-2.077699	-0.000059
6	0	5.894624	1.879688	-0.000133
6	0	4.730345	-0.295793	0.000032
6	0	-3.654242	-2.779505	-0.000184
8	0	-1.29685	-2.790068	0.00002
6	0	-3.66656	0.007871	0.000047
6	0	-4.851526	-2.090424	-0.000188
6	0	-4.892885	-0.675881	-0.000061
6	0	5.951195	0.454928	-0.000001
6	0	-6.03026	1.465066	0.000104
6	0	-4.769058	2.160927	0.000209
8	0	-4.596023	3.371107	0.00033
6	0	-7.452914	-0.58457	-0.000133
6	0	4.83303	-1.713492	0.000118
6	0	7.263152	-1.598177	0.000184
6	0	6.063917	-2.344891	0.000196
6	0	-6.116114	0.102696	-0.000029
6	0	7.200312	-0.219804	0.000083
1	0	1.569623	1.931391	-0.000112
1	0	2.207576	-1.385788	0.000215
1	0	-1.227124	1.186802	-0.000049
1	0	4.653661	3.633589	-0.000325
1	0	6.826764	2.437885	-0.000152
1	0	-3.63011	-3.863539	-0.000259
1	0	-0.527398	-2.151041	0.000307
1	0	-5.78008	-2.64986	-0.000281
1	0	-6.915532	2.089979	0.000131
1	0	-8.265174	0.144361	-0.000158
1	0	-7.563526	-1.225077	0.881804
1	0	-7.563426	-1.225028	-0.882116

1	0	3.942439	-2.33035	0.000115
1	0	8.222242	-2.106617	0.00025
1	0	6.105045	-3.430169	0.000258
1	0	8.110535	0.373961	0.000062

2. CHN-S-1 (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-3.61012	1.36903	0.000349
7	0	-0.050086	-0.540787	0.000237
8	0	2.31293	2.482708	0.000028
6	0	3.416135	1.849602	-0.000162
6	0	2.280568	-0.332868	0.00028
6	0	3.474442	0.39029	0.000198
6	0	-2.434094	-0.675052	-0.000033
7	0	1.071876	0.232939	0.000389
6	0	-1.192387	0.073931	0.000158
6	0	4.672759	2.571789	-0.000863
6	0	-2.471012	-2.094158	-0.000319
6	0	5.865905	1.919074	-0.001016
6	0	4.767212	-0.299163	0.000225
6	0	-3.699709	-2.778635	-0.000578
8	0	-1.346088	-2.831104	-0.000337
6	0	-3.673785	0.006236	0.000037
6	0	-4.888373	-2.074335	-0.000522
6	0	-4.909559	-0.659949	-0.000208
6	0	5.960737	0.481552	-0.000435
6	0	-6.01611	1.497409	0.000216
6	0	-4.745051	2.17547	0.000473
8	0	-4.554408	3.382699	0.000785
6	0	-7.467848	-0.531683	-0.000376
6	0	4.908136	-1.706665	0.000943
6	0	7.332451	-1.531856	0.000192
6	0	6.159933	-2.30869	0.000907
6	0	-6.121599	0.136619	-0.000115
6	0	7.224674	-0.150261	-0.000451
1	0	1.066048	1.272682	0.000391
1	0	2.265245	-1.416933	0.000196
1	0	-1.248687	1.162354	0.000173
1	0	4.619265	3.656066	-0.001254
1	0	6.792736	2.488126	-0.001564
1	0	-3.689299	-3.862869	-0.000789
1	0	-0.563979	-2.222412	0.000014
1	0	-5.824122	-2.621569	-0.000709
1	0	-6.892246	2.135038	0.000304
1	0	-8.269879	0.208466	-0.000328

1	0	-7.587343	-1.170733	0.881454
1	0	-7.587163	-1.170423	-0.882454
1	0	4.035159	-2.349583	0.001597
1	0	8.307343	-2.00918	0.000181
1	0	6.228067	-3.392671	0.001466
1	0	8.117256	0.469985	-0.000958

3. CHN-S-2 (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-3.687882	1.375207	-0.000518
7	0	-0.045633	-0.400193	0.000502
8	0	2.411117	2.606256	0.001381
6	0	3.52173	1.84411	0.000897
6	0	2.218148	-0.262666	0.000185
6	0	3.481627	0.433471	0.000227
6	0	-2.423773	-0.625153	0.000385
7	0	1.081488	0.374089	0.000397
6	0	-1.246731	0.148559	0.000257
6	0	4.754997	2.541701	0.001153
6	0	-2.358061	-2.085505	0.000904
6	0	5.937874	1.849152	0.000692
6	0	4.732288	-0.303703	-0.00033
6	0	-3.614329	-2.794139	0.00103
8	0	-1.241251	-2.694855	0.00124
6	0	-3.697371	0.014997	-0.000015
6	0	-4.809554	-2.128842	0.000633
6	0	-4.89582	-0.698378	0.000076
6	0	5.966931	0.423918	-0.000075
6	0	-6.093227	1.410308	-0.000962
6	0	-4.858009	2.140681	-0.001028
8	0	-4.707696	3.355444	-0.001467
6	0	-7.454012	-0.682284	-0.000376
6	0	4.809018	-1.722887	-0.001153
6	0	7.240815	-1.652771	-0.0014
6	0	6.028087	-2.376825	-0.001668
6	0	-6.135127	0.040905	-0.000425
6	0	7.203369	-0.273656	-0.000618
1	0	1.61479	2.015517	0.001109
1	0	2.216949	-1.351689	0.000032
1	0	-1.285305	1.232804	-0.000056
1	0	4.730143	3.626209	0.001706
1	0	6.880336	2.389549	0.000898
1	0	-3.577353	-3.878573	0.001439
1	0	-0.038974	-1.444754	0.000833
1	0	-5.730251	-2.702742	0.000744

1	0	-6.998988	2.005008	-0.001367
1	0	-8.285469	0.024802	-0.000773
1	0	-7.54846	-1.325342	0.881635
1	0	-7.548166	-1.325993	-0.881945
1	0	3.909281	-2.326398	-0.001427
1	0	8.190216	-2.178954	-0.001821
1	0	6.048652	-3.4626	-0.002296
1	0	8.124084	0.303513	-0.000417

4. CHN-D (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-3.723796	1.387105	0.088233
7	0	-0.073801	-0.38942	-0.051985
8	0	2.334151	2.473265	-0.19424
6	0	3.439843	1.837894	-0.134353
6	0	2.282798	-0.320535	0.003952
6	0	3.48821	0.38451	-0.025812
6	0	-2.428738	-0.585893	-0.03569
7	0	1.10251	0.297334	-0.05489
6	0	-1.251953	0.197524	-0.011341
6	0	4.695749	2.55317	-0.175263
6	0	-2.335757	-2.0369	-0.113349
6	0	5.88513	1.894971	-0.10914
6	0	4.773599	-0.311211	0.046211
6	0	-3.569141	-2.772956	-0.142977
8	0	-1.195361	-2.619963	-0.153673
6	0	-3.709456	0.028743	0.012902
6	0	-4.779781	-2.132552	-0.0944
6	0	-4.894245	-0.708953	-0.013711
6	0	5.971201	0.461929	0.003754
6	0	-6.130276	1.372833	0.11924
6	0	-4.908616	2.127023	0.145635
8	0	-4.783063	3.34233	0.212304
6	0	-7.452504	-0.741961	0.015655
6	0	4.903097	-1.715076	0.157124
6	0	7.328106	-1.553164	0.181188
6	0	6.150653	-2.321779	0.222947
6	0	-6.147814	0.005638	0.041853
6	0	7.230779	-0.175281	0.072537
1	0	1.164526	1.346943	-0.126638
1	0	2.250138	-1.402285	0.074714
1	0	-1.292595	1.281107	0.037721
1	0	4.648637	3.634292	-0.259124
1	0	6.815129	2.457629	-0.141088
1	0	-3.509868	-3.854602	-0.202821

1	0	-0.141963	-1.457148	-0.104491
1	0	-5.688126	-2.725096	-0.117431
1	0	-7.046566	1.949439	0.164391
1	0	-8.297084	-0.052441	0.06531
1	0	-7.523158	-1.436459	0.860096
1	0	-7.545324	-1.335854	-0.900358
1	0	4.025584	-2.350991	0.194296
1	0	8.299425	-2.034756	0.233963
1	0	6.212038	-3.402751	0.307794
1	0	8.127509	0.437831	0.039021

5. CHN-O (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	-3.502363	1.335519	-0.00162
7	0	-0.002255	-0.600473	0.00044
8	0	2.465153	2.665719	0.000744
6	0	3.584792	1.896639	0.001056
6	0	2.183862	-0.193494	0.001315
6	0	3.465809	0.497054	0.000104
6	0	-2.441555	-0.777291	-0.000194
7	0	1.011736	0.363441	-0.002508
6	0	-1.174298	-0.052271	-0.001768
6	0	4.851346	2.532955	0.002834
6	0	-2.585693	-2.186146	0.001134
6	0	6.005098	1.79262	0.003314
6	0	4.688572	-0.291266	-0.000557
6	0	-3.858469	-2.784963	0.002224
8	0	-1.470602	-2.952022	0.001197
6	0	-3.643664	-0.023701	-0.000424
6	0	-5.002502	-2.010001	0.001978
6	0	-4.92566	-0.602252	0.00065
6	0	5.96171	0.372318	0.001413
6	0	-5.893636	1.620462	-0.000869
6	0	-4.580059	2.212004	-0.001934
8	0	-4.312271	3.405123	-0.00319
6	0	-7.471117	-0.311507	0.001481
6	0	4.708904	-1.716415	-0.003756
6	0	7.14255	-1.759432	-0.00139
6	0	5.895737	-2.424879	-0.004065
6	0	-6.084998	0.270142	0.000379
6	0	7.166228	-0.381767	0.001149
1	0	2.714917	3.601907	0.002759
1	0	2.20747	-1.282497	0.006446
1	0	-1.244771	1.035518	-0.005007
1	0	4.893673	3.61907	0.004019

1	0	6.970016	2.2915	0.004915
1	0	-3.933808	-3.86831	0.003203
1	0	-1.716749	-3.889724	0.001624
1	0	-5.970386	-2.497559	0.002847
1	0	-6.726569	2.313513	-0.001145
1	0	-8.223888	0.478767	0.000862
1	0	-7.631103	-0.940457	0.884215
1	0	-7.631724	-0.942426	-0.879725
1	0	3.786992	-2.283117	-0.006644
1	0	8.066633	-2.329047	-0.001624
1	0	5.864761	-3.510539	-0.006611
1	0	8.111092	0.155037	0.002846

6. CHN (S_1)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	3.627657	1.378381	0.000037
7	0	0.013156	-0.55103	-0.00006
8	0	-2.271054	2.469684	-0.000053
6	0	-3.428792	1.802612	-0.000034
6	0	-2.248873	-0.402549	-0.000036
6	0	-3.456777	0.350561	-0.000026
6	0	2.40664	-0.64418	-0.000062
7	0	-1.059862	0.21918	-0.00005
6	0	1.196587	0.092632	-0.000072
6	0	-4.612516	2.556162	-0.000023
6	0	2.442785	-2.086695	-0.000099
6	0	-5.845745	1.932449	-0.000006
6	0	-4.75827	-0.291329	-0.000007
6	0	3.661468	-2.777088	-0.000058
8	0	1.304494	-2.798548	-0.000194
6	0	3.675037	0.014366	0.000004
6	0	4.865452	-2.088411	0.00001
6	0	4.896832	-0.668191	0.00004
6	0	-5.949052	0.511216	0.000001
6	0	6.029926	1.477329	0.000138
6	0	4.76788	2.171102	0.000103
8	0	4.593705	3.383069	0.000126
6	0	7.456432	-0.56961	0.000147
6	0	-4.912134	-1.699918	0.000005
6	0	-7.329002	-1.506697	0.000027
6	0	-6.170797	-2.297564	0.000022
6	0	6.11749	0.113918	0.000108
6	0	-7.212676	-0.118875	0.000017
1	0	-1.519546	1.78906	-0.000065
1	0	-2.259636	-1.488946	-0.000031

1	0	1.217736	1.180026	-0.000054
1	0	-4.527795	3.637815	-0.00003
1	0	-6.75484	2.526311	0.000001
1	0	3.639395	-3.861679	-0.000088
1	0	0.533914	-2.15068	-0.000269
1	0	5.795224	-2.644987	0.000037
1	0	6.915211	2.102457	0.000189
1	0	8.267183	0.161116	0.000201
1	0	7.568273	-1.210165	-0.881621
1	0	7.568199	-1.210213	0.88189
1	0	-4.042798	-2.345547	0.000002
1	0	-8.310058	-1.970597	0.000039
1	0	-6.248288	-3.379968	0.00003
1	0	-8.10501	0.500833	0.000021

7. CHN-S-1 (S_1)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	3.555725	1.370022	0.000053
7	0	0.034365	-0.695803	-0.000065
8	0	-2.206833	2.353746	0.000135
6	0	-3.351883	1.792094	0.000126
6	0	-2.299426	-0.494946	-0.000036
6	0	-3.476469	0.321971	0.00001
6	0	2.428745	-0.705797	-0.000065
7	0	-1.078093	0.036083	-0.000043
6	0	1.189223	-0.014198	-0.000069
6	0	-4.556732	2.578907	0.0002
6	0	2.528562	-2.140379	-0.000116
6	0	-5.794883	1.999168	0.000155
6	0	-4.77777	-0.273013	-0.000054
6	0	3.775793	-2.775457	-0.000083
8	0	1.424759	-2.914054	-0.000219
6	0	3.664733	0.009796	0.000007
6	0	4.949396	-2.034878	-0.000008
6	0	4.917091	-0.61641	0.000036
6	0	-5.948483	0.573148	0.000023
6	0	5.950856	1.579655	0.000151
6	0	4.658905	2.214925	0.000124
8	0	4.427828	3.417287	0.000157
6	0	7.468758	-0.400283	0.000143
6	0	-4.984466	-1.68909	-0.000197
6	0	-7.387653	-1.396761	-0.000177
6	0	-6.254966	-2.235192	-0.000256
6	0	6.100346	0.221816	0.000111
6	0	-7.225222	-0.012935	-0.000041

1	0	-1.078421	1.085376	0.000006
1	0	-2.337078	-1.575997	-0.000056
1	0	1.187931	1.074054	-0.000036
1	0	-4.435597	3.657703	0.000292
1	0	-6.690219	2.61463	0.000216
1	0	3.80149	-3.859981	-0.000123
1	0	0.623587	-2.325011	-0.000277
1	0	5.902408	-2.55054	0.000013
1	0	6.806644	2.244512	0.000208
1	0	8.245964	0.366096	0.000208
1	0	7.60913	-1.035497	-0.881499
1	0	7.609055	-1.035572	0.881743
1	0	-4.138364	-2.364705	-0.000267
1	0	-8.384107	-1.82668	-0.000224
1	0	-6.377074	-3.313403	-0.000366
1	0	-8.097818	0.634197	0.000016

8. CHN-S-2 (S_1)

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	3.707388	1.387235	-0.000132
7	0	0.02542	-0.332581	0.000035
8	0	-2.428101	2.597563	-0.000181
6	0	-3.544612	1.843133	-0.000115
6	0	-2.247006	-0.280228	0.000067
6	0	-3.492561	0.411013	0.000025
6	0	2.431152	-0.587956	0.00001
7	0	-1.088347	0.384334	0.000017
6	0	1.25199	0.217095	-0.000015
6	0	-4.770639	2.532453	-0.0002
6	0	2.376201	-2.059039	0.000099
6	0	-5.965062	1.843491	-0.000142
6	0	-4.756505	-0.312399	0.000107
6	0	3.62631	-2.782448	0.00012
8	0	1.265018	-2.671622	0.000161
6	0	3.696229	0.01564	-0.000048
6	0	4.838609	-2.138127	0.00006
6	0	4.916461	-0.716284	-0.000027
6	0	-5.990584	0.419614	0.000015
6	0	6.115956	1.381768	-0.000169
6	0	4.880191	2.124046	-0.000191
8	0	4.765295	3.341793	-0.000257
6	0	7.475471	-0.714152	-0.000071
6	0	-4.834207	-1.728155	0.000279
6	0	-7.262248	-1.664517	0.000248
6	0	-6.055108	-2.389407	0.000347

6	0	6.155231	0.008481	-0.00009
6	0	-7.22309	-0.280269	0.000087
1	0	-1.636335	1.993358	-0.000115
1	0	-2.226581	-1.367495	0.000131
1	0	1.302103	1.297399	-0.000076
1	0	-4.745185	3.617327	-0.000314
1	0	-6.905544	2.386667	-0.000215
1	0	3.565876	-3.865851	0.000187
1	0	0.016028	-1.371229	0.000092
1	0	5.754283	-2.717756	0.000079
1	0	7.023169	1.974193	-0.000218
1	0	8.304074	-0.00393	-0.000143
1	0	7.572351	-1.355424	-0.882505
1	0	7.572394	-1.355292	0.882455
1	0	-3.932768	-2.329061	0.000369
1	0	-8.214005	-2.18651	0.000302
1	0	-6.073608	-3.474948	0.000479
1	0	-8.145629	0.294025	0.000014

9. CHN-D (S_1)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
8	0	3.656917	1.390172	-0.008873
7	0	0.044777	-0.502823	0.002361
8	0	-2.232878	2.354174	0.017802
6	0	-3.382201	1.779841	0.013524
6	0	-2.315207	-0.471672	-0.00258
6	0	-3.497322	0.315915	0.002196
6	0	2.439335	-0.627709	0.003033
7	0	-1.120377	0.131079	0.002586
6	0	1.242171	0.12749	-0.000311
6	0	-4.587288	2.559049	0.019629
6	0	2.42523	-2.100577	0.010528
6	0	-5.821001	1.968992	0.013854
6	0	-4.803307	-0.294979	-0.004147
6	0	3.693068	-2.782985	0.014162
8	0	1.324824	-2.742743	0.013615
6	0	3.694096	0.019381	-0.00117
6	0	4.883143	-2.099571	0.010196
6	0	4.922449	-0.671478	0.002116
6	0	-5.97107	0.541896	0.001593
6	0	6.061364	1.463935	-0.011124
6	0	4.80511	2.16751	-0.014431
8	0	4.646906	3.381851	-0.021572
6	0	7.48083	-0.590967	0.000187
6	0	-4.999752	-1.704934	-0.016067

6	0	-7.407921	-1.429737	-0.016826
6	0	-6.270509	-2.258817	-0.022301
6	0	6.140663	0.093703	-0.003027
6	0	-7.250232	-0.047749	-0.005013
1	0	-1.213312	1.204655	0.009396
1	0	-2.325592	-1.554233	-0.010091
1	0	1.245403	1.209377	-0.005347
1	0	-4.475997	3.638851	0.028629
1	0	-6.718854	2.58117	0.018445
1	0	3.669097	-3.867898	0.020037
1	0	0.104529	-1.546925	0.006296
1	0	5.816159	-2.65172	0.01309
1	0	6.951062	2.082524	-0.015414
1	0	8.29009	0.141394	-0.003442
1	0	7.59516	-1.234258	-0.878881
1	0	7.595353	-1.225702	0.885412
1	0	-4.149848	-2.377087	-0.020655
1	0	-8.401979	-1.865441	-0.021793
1	0	-6.384604	-3.338202	-0.031439
1	0	-8.123514	0.598852	-0.000774