Supporting information

Table S1. Cartesian coordinates of optimized structure of CPDS-H_2O clusters in the CT state. Coordinates are in unit of Å.

	on-ring 1			side		
C	-0.71069	0.698791	-0.230282	-0.225326	-0.848401	-0.20377
Si	0.924678	1.207106	0.339458	1.479499	-1.197444	0.272136
Si	2.692391	-0.778067	-0.543478	2.827685	1.215	-0.183413
C	1.736997	2.666426	-0.539957	2.079063	-1.494911	2.044243
H	1.096533	3.538549	-0.36055	1.696915	-2.477512	2.348761
H	1.773846	2.520815	-1.620947	1.665699	-0.760676	2.737893
H	2.733173	2.902826	-0.16084	3.168147	-1.518855	2.137817
C	1.447541	1.197102	2.154188	2.493739	-2.273119	-0.899133
H	0.911614	2.023401	2.638968	2.025419	-3.264611	-0.910486
H	1.136232	0.273669	2.643669	2.462563	-1.897901	-1.923324
H	2.517089	1.367328	2.302075	3.529717	-2.401831	-0.579902
C	2.221682	-1.046986	-2.341629	2.377301	2.367645	1.230777
H	1.227807	-1.478613	-2.452383	1.307274	2.569741	1.278121
H	2.257275	-0.11129	-2.902453	2.700361	1.959406	2.19027
H	2.950017	-1.734975	-2.785815	2.897143	3.320151	1.078335
C	2.441947	-2.230449	0.618386	2.209701	1.719296	-1.881772
H	1.395613	-2.391634	0.877916	1.128539	1.855001	-1.89577
H	2.994729	-2.069874	1.546128	2.475054	0.97406	-2.633693
H	2.831295	-3.134809	0.13837	2.684535	2.666855	-2.159676
C	4.369482	0.055394	-0.351956	4.641518	0.710964	-0.155459
H	4.472217	0.923865	-1.00434	4.933302	0.292654	0.809677
H	4.557839	0.360724	0.678847	4.876201	-0.010534	-0.939612
H	5.143147	-0.669092	-0.630987	5.249985	1.605715	-0.328991
C	-1.142274	-0.647933	-0.555049	-0.915654	0.417672	-0.028932
C	-1.789334	1.641859	0.050424	-1.091379	-2.019514	-0.288434
C	-2.467109	-0.996095	-0.640371	-2.281814	0.517738	-0.024342
C	-3.11222	1.290435	-0.024806	-2.459606	-1.923647	-0.266856
H	-0.410516	-1.420043	-0.758178	-0.348847	1.334795	0.076925
H	-1.555801	2.67086	0.308725	-0.657228	-3.00789	-0.407057
H	-2.741912	-2.004927	-0.919979	-2.76132	1.482616	0.069372
H	-3.878593	2.030074	0.165418	-3.0653	-2.814073	-0.371674
C	-3.500137	-0.042363	-0.373269	-3.099156	-0.652285	-0.140012
C	-4.874529	-0.414636	-0.446126	-4.518129	-0.531472	-0.127215
N	-5.975826	-0.718017	-0.501112	-5.655428	-0.401187	-0.114606
H	-1.078349	-1.341796	1.863479	-5.47596	2.124479	-0.285046
O	-0.479559	-1.751596	2.477504	-5.149319	2.778551	0.319077
H	-1.033109	-2.251986	3.059603	-5.271779	2.362725	1.160979

Table S1. continued.

	Linear			on-ring 2		
C	0.037601	0.610494	-0.232559	0.644171	0.011802	-0.368365
Si	-1.62988	1.162142	0.183167	-0.865955	0.959005	0.035308
Si	-3.21721	-1.127287	-0.102792	-2.831637	-1.033983	-0.055205
C	-2.207184	1.657042	1.917088	-1.314176	1.667669	1.728435
H	-1.727089	2.615803	2.150434	-0.702874	2.564085	1.872366
H	-1.876889	0.941031	2.671629	-1.081644	0.965003	2.53105
H	-3.288407	1.80045	1.992167	-2.367648	1.955493	1.792803
C	-2.518539	2.236215	-1.086794	-1.545732	2.056836	-1.333137
H	-1.952909	3.172139	-1.167799	-0.871851	2.917278	-1.403612
H	-2.515116	1.778956	-2.077594	-1.552164	1.553001	-2.300906
H	-3.539398	2.492487	-0.797219	-2.542468	2.43968	-1.106807
C	-2.888757	-2.203228	1.402423	-2.804068	-1.984655	1.570059
H	-1.84359	-2.502678	1.480399	-1.855426	-2.497062	1.732507
H	-3.176304	-1.691249	2.322668	-2.996033	-1.325674	2.41914
H	-3.497561	-3.110403	1.31804	-3.597227	-2.740465	1.545876
C	-2.647123	-1.823322	-1.749497	-2.281558	-2.017029	-1.55818
H	-1.582731	-2.057272	-1.74485	-1.260155	-2.379925	-1.440754
H	-2.843579	-1.121016	-2.561536	-2.326712	-1.409302	-2.463845
H	-3.206055	-2.743428	-1.953288	-2.94855	-2.876307	-1.688902
C	-4.969564	-0.440982	-0.134775	-4.456703	-0.109416	-0.301289
H	-5.220657	0.078496	0.791867	-4.672661	0.558465	0.535221
H	-5.126301	0.23744	-0.974836	-4.456674	0.472641	-1.224402
H	-5.66568	-1.279996	-0.246091	-5.27092	-0.840114	-0.363989
C	0.600651	-0.697893	0.046999	1.051052	-1.160783	0.3873
C	1.013606	1.685647	-0.377676	1.740921	0.793887	-0.921849
C	1.951032	-0.92302	0.094677	2.360727	-1.548207	0.506466
C	2.365463	1.464032	-0.311808	3.057309	0.418582	-0.786374
H	-0.053112	-1.548158	0.20029	0.298493	-1.780516	0.862896
H	0.678601	2.699209	-0.577171	1.524238	1.67791	-1.510536
H	2.327549	-1.922221	0.268934	2.613174	-2.453722	1.041942
H	3.055022	2.284244	-0.461084	3.836758	0.994173	-1.269427
C	2.881073	0.151714	-0.078237	3.411404	-0.763091	-0.068037
C	4.283617	-0.082528	-0.013732	4.777453	-1.151068	0.072939
N	5.409582	-0.273793	0.038233	5.872264	-1.46036	0.186074
H	7.529364	-0.681576	0.343675	1.612227	4.396503	0.306877
O	8.448972	-0.868283	0.190614	1.193501	3.604794	0.612667
H	8.514004	-0.872439	-0.753085	1.885758	2.955552	0.639397

Table S1. continued.

	disilanyl-side		
C	-1.063401	-0.41571	-0.185163
Si	0.669094	-0.870738	-0.00448
Si	2.064836	1.555058	-0.092626
C	1.412614	-1.544765	1.59796
H	1.017574	-2.561021	1.725569
H	1.090488	-0.96552	2.465088
H	2.502235	-1.606004	1.567724
C	1.530978	-1.680992	-1.471222
H	1.01195	-2.628363	-1.661271
H	1.438475	-1.084456	-2.380609
H	2.578709	-1.904629	-1.265129
C	1.860326	2.314473	1.614916
H	0.812395	2.460336	1.878886
H	2.332477	1.694395	2.379193
H	2.35279	3.293261	1.622248
C	1.252408	2.490084	-1.503747
H	0.209567	2.72718	-1.297518
H	1.298329	1.915201	-2.430529
H	1.801037	3.426033	-1.658918
C	3.832609	1.038679	-0.471028
H	4.201839	0.276789	0.216104
H	3.920026	0.658307	-1.490483
H	4.472712	1.924195	-0.383946
C	-1.681806	0.826599	0.226299
C	-1.983124	-1.513156	-0.442062
C	-3.042006	0.975915	0.313692
C	-3.343488	-1.368507	-0.3398
H	-1.067744	1.684755	0.471829
H	-1.600192	-2.481752	-0.750424
H	-3.461889	1.930243	0.603276
H	-3.992212	-2.204251	-0.566741
C	-3.923282	-0.116488	0.035548
C	-5.336331	0.038731	0.136143
N	-6.470536	0.165445	0.216458
H	5.597388	-2.320167	-0.165289
O	4.827449	-2.267482	0.383389
H	4.790206	-3.102456	0.828887