Supporting Information

Solution processed organic solar cells based on A-D-D'-D-A Small Molecule with Benzo[1,2-b:4,5-b′]dithiophene donor unit and ethylrhodanine acceptor unit having 6 % light to energy conversion efficiency

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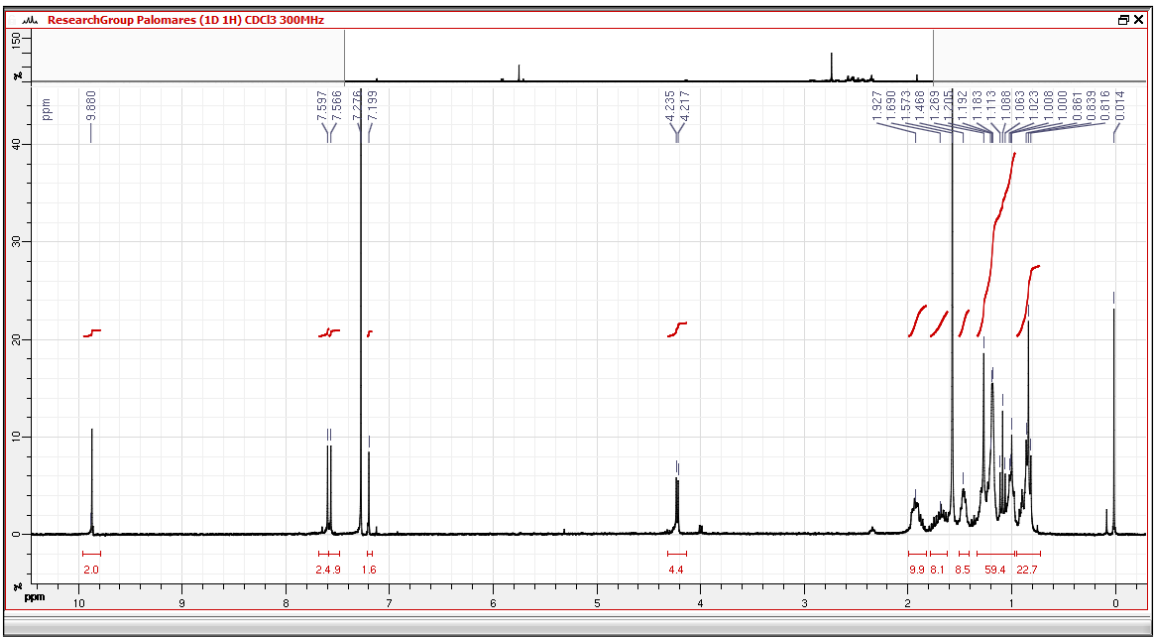


Fig. S1 ^{1}H NMR spectra of compound **3** recorded in $CDCl_3$.

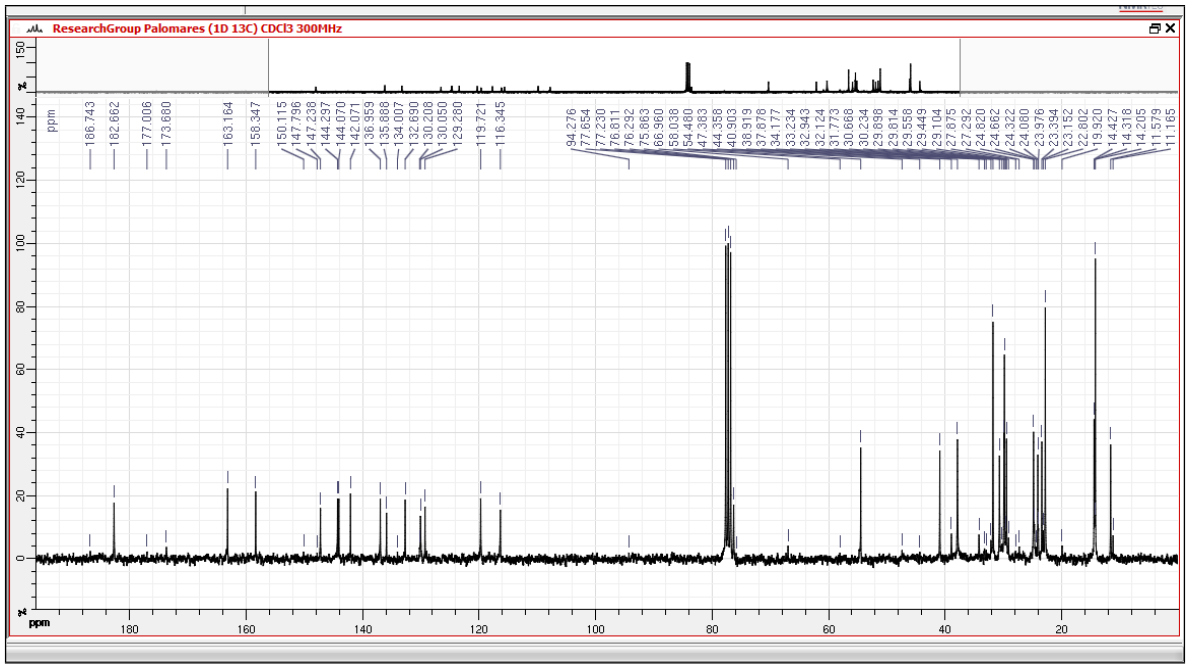


Fig. S2 ^{13}C NMR spectra of compound **3** recorded in $CDCl_3$.

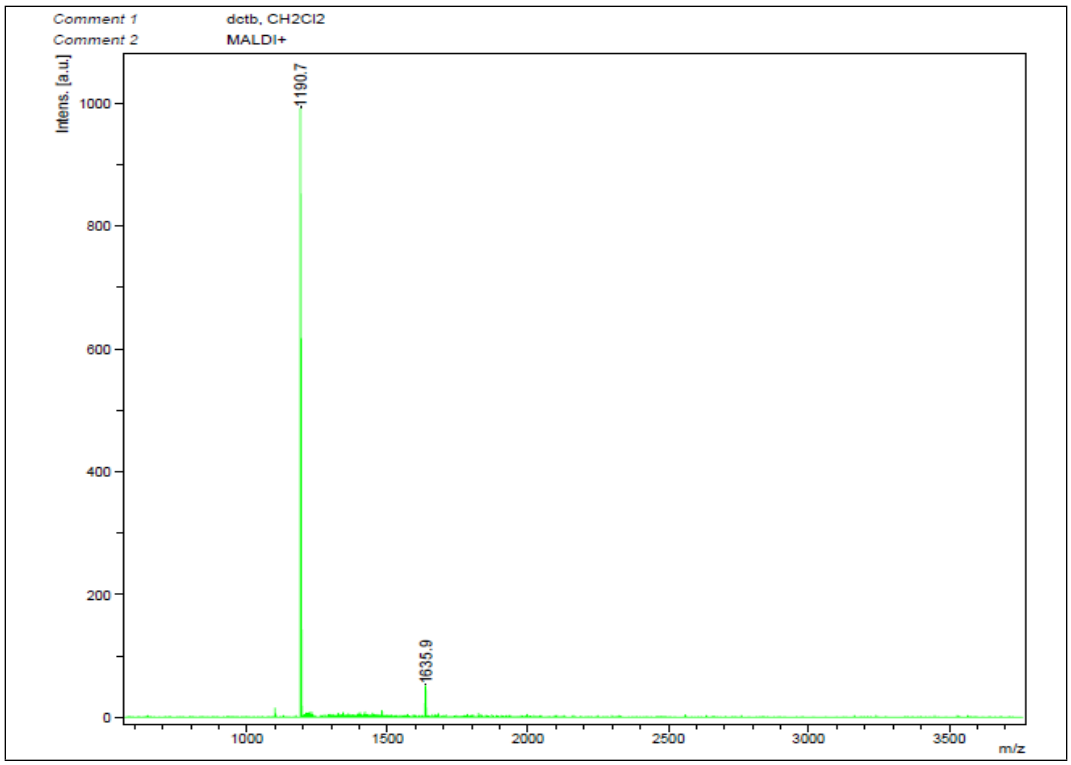


Fig. S3 MALDI-TOF spectrum of compound **3**

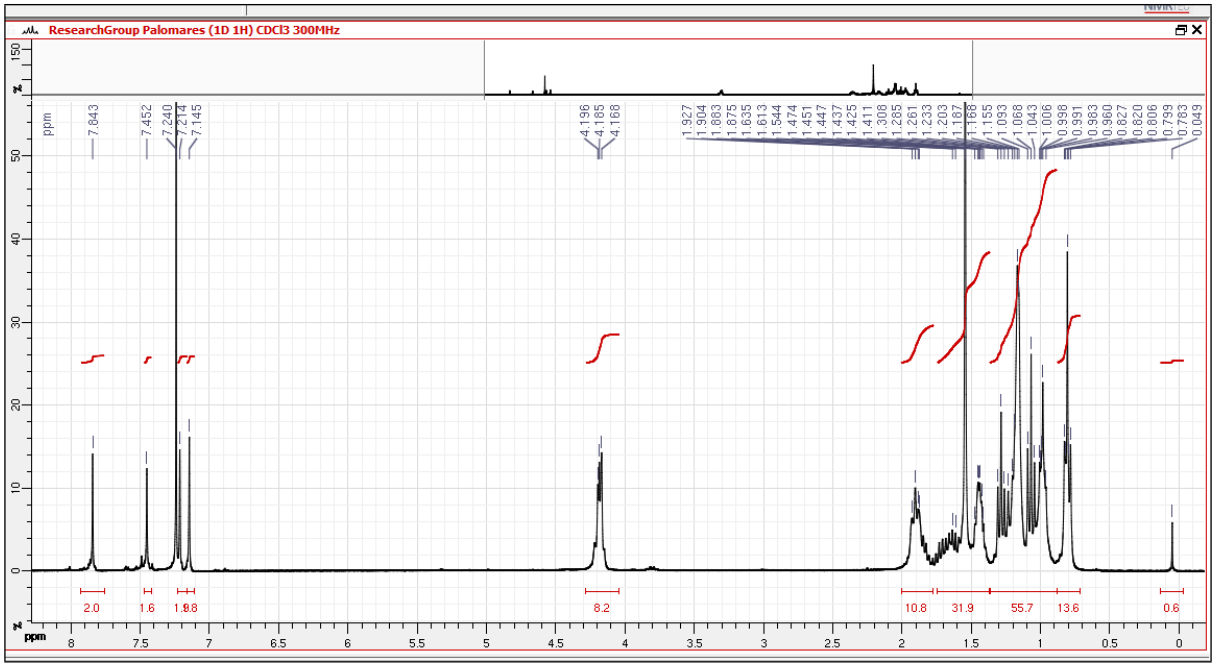


Fig. S4 ^{1}H NMR spectra of compound **BDT(CDTRH)$_2$** recorded in $CDCl_3$.

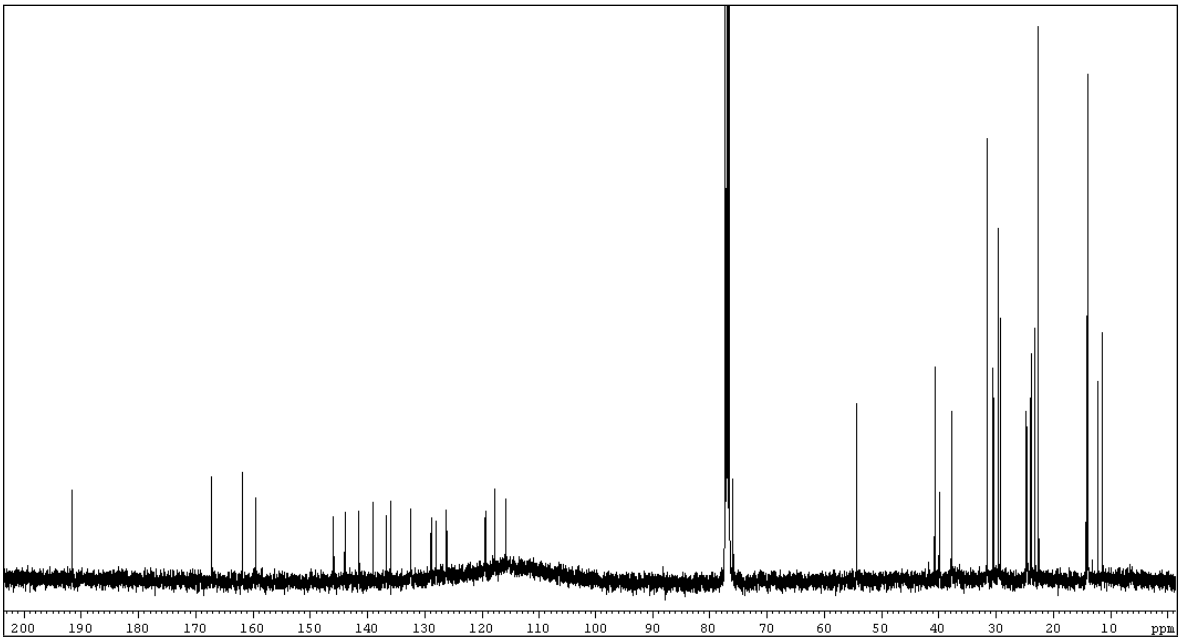


Fig. S5 ^{13}C NMR spectra of compound **BDT(CDTRH)$_2$** recorded in $CDCl_3$.

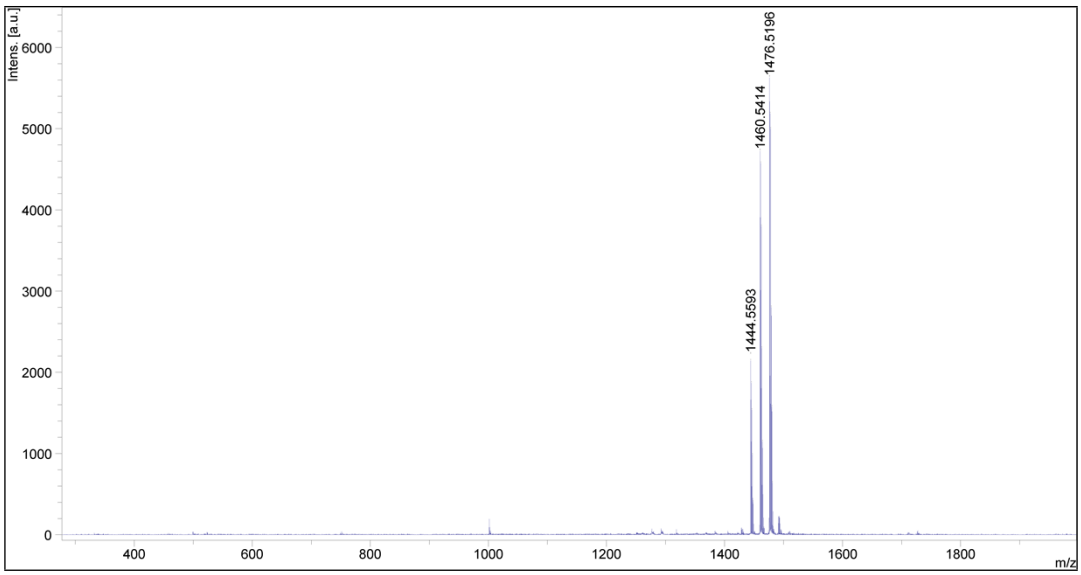


Fig. S6 MALDI-TOF spectrum of compound **BDT(CDTRH)$_2$.**

Total and Partial Density of States

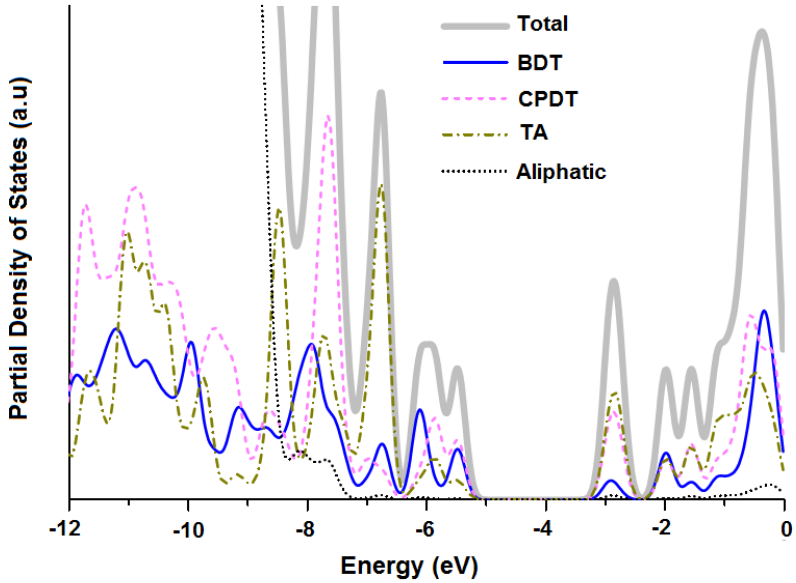


Figure S7. Total and partial density of states of the **BDT(CDTRH)$_2$** (calculated using the M06 functional).

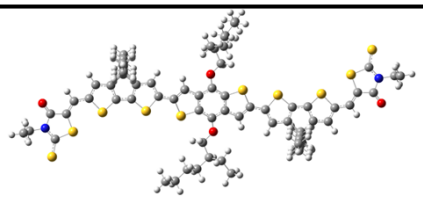
Energies of BDT(CDTRH)$_2$ isomers

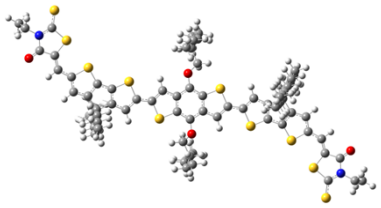
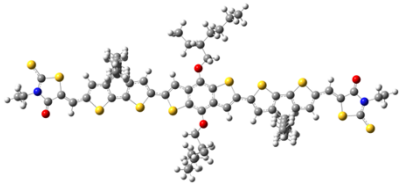
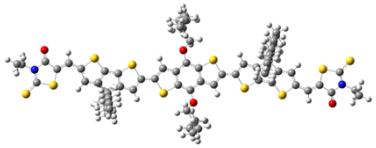
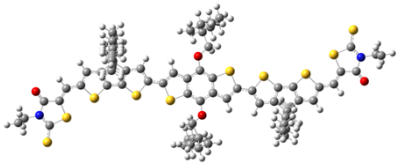
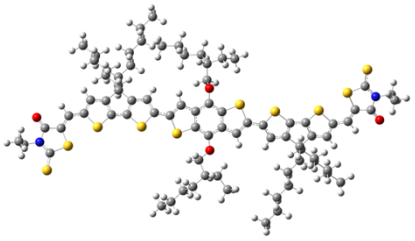
The energetically lowest isomers of **BDT(CDTRH)$_2$** are shown in Table S1. We have included the absolute energy of the structures along the energy difference from the lowest energy structure (isomer 1). These values correspond to the DFT/PBE/TZVP level of theory. Isomer 1 was used as the main structure discussed in the text. The Cartesian coordinates for each of the structures are given in Table S2.

Alteration of alkyl group configurations, which have also been considered in these isomers, can have an impact on the energy of the structure even up to a few kcal mol^{-1}. Alkyl configurations may also favor rotations of thiophene groups through steric repulsions, in which case the overall planarity of the structure is altered. In the provided density of states diagram contributions from the alkyl groups show up at low energies (first significant contributions is around –9 eV). Alkyl groups are not expected to contribute to states involved in excitations in the visible and near (and perhaps even middle-) ultra-violet region. Thus, insofar as the backbone of the structure remains more or less unaltered, isomers from purely alkyl reconfigurations should not impact the UV/Vis spectrum. We note that the calculations must be performed on structures that include the full alkyl groups (as performed here) so that the effects of the alkyl configurations can be accounted for and be assessed. This would not be the case if the alkyl groups had been truncated to simple methyl groups (a tactic followed to increase computational efficiency, which however in many cases has merits).

In all of the isomers considered alkyl groups extend out of main body (thiophene chain) plane. This does not favor pi-stacking of the molecule, and ultimately affects the crystallinity of the thin-films.

Table S1. Energy of energetically low **BDT(CDTRH)$_2$** isomers (at the DFT/PBE/TZVP level of theory). Absolute energy and energy difference relative to isomer 1.

isomer	Energy (Eh)	ΔE (kcal mol^{-1})	STRUCTURE
1	-7498.47445	0.00	

2	-7498.47419	+0.16	
3	-7498.47293	+0.95	
4	-7498.47275	+1.07	
5	-7498.47132	+1.96	
6	-7498.47111	+2.09	

Coordinates of the isomers

Table S2. Cartesian coordinates of **BDT(CDTRH)$_2$** isomers 1,2 and 3, optimized at the DFT/PBE/TZVP level of theory (units in Ångströms).

isomer 1				**isomer 2**				**isomer 3**			
atom	**x**	**y**	**z**	**atom**	**x**	**y**	**z**	**atom**	**x**	**y**	**z**
c	1.208	0.693	0.017	c	-0.699	-1.208	0.003	c	1.203	0.706	-0.012
c	1.223	-0.726	-0.173	c	0.720	-1.158	0.182	c	1.225	-0.714	-0.192

c	0.042	-1.470	-0.236	c	1.410	0.056	0.219	c	0.048	-1.462	-0.263
c	-1.177	-0.761	-0.102	c	0.641	1.242	0.111	c	-1.175	-0.757	-0.144
c	-1.192	0.659	0.089	c	-0.780	1.191	-0.047	c	-1.199	0.664	0.035
c	-0.011	1.402	0.152	c	-1.465	-0.023	-0.124	c	-0.021	1.413	0.100
c	2.514	1.258	0.035	c	-1.208	-2.536	0.020	c	2.506	1.277	0.018
c	3.527	0.346	-0.169	c	-0.251	-3.507	0.223	c	3.525	0.367	-0.168
h	2.691	2.316	0.220	h	-2.269	-2.753	-0.095	h	2.675	2.337	0.193
c	-2.482	-1.328	-0.120	c	1.137	2.572	0.185	c	-2.477	-1.331	-0.161
c	-3.497	-0.417	0.077	c	0.163	3.545	0.116	c	-3.497	-0.423	0.028
h	-2.654	-2.388	-0.301	h	2.197	2.792	0.303	h	-2.643	-2.393	-0.329
o	-0.068	-2.816	-0.461	o	2.752	0.228	0.431	o	-0.051	-2.809	-0.488
o	0.102	2.748	0.379	s	1.371	-2.791	0.394	o	0.087	2.762	0.304
s	2.884	-1.296	-0.398	s	-1.458	2.826	-0.063	s	2.891	-1.279	-0.389
s	-2.856	1.225	0.306	c	1.231	7.278	0.374	s	-2.867	1.225	0.241
c	-7.396	-0.454	0.047	c	-0.156	7.258	0.194	c	-7.399	-0.529	0.046
c	-6.961	-1.773	0.219	c	-0.719	8.676	0.175	c	-6.935	-1.839	0.208
c	-8.150	-2.724	0.331	c	0.562	9.484	0.373	c	-8.099	-2.817	0.331
c	-9.305	-1.737	0.188	c	1.670	8.628	0.483	c	-9.276	-1.855	0.208
c	-8.820	-0.429	0.029	c	0.909	10.831	0.476	c	-8.825	-0.534	0.046
c	-10.699	-1.803	0.174	c	2.287	11.040	0.666	c	-10.667	-1.965	0.219
c	-11.315	-0.550	0.004	c	0.308	4.968	0.174	c	-11.321	-0.730	0.062
c	-4.910	-0.665	0.110	c	-0.673	5.958	0.080	c	-4.907	-0.690	0.075
c	-5.565	-1.890	0.262	s	3.158	9.483	0.714	c	-5.536	-1.928	0.233
s	-10.089	0.739	-0.140	s	1.920	5.685	0.411	s	-10.129	0.592	-0.099
s	-6.074	0.663	-0.088	h	-1.726	5.716	-0.064	s	-6.100	0.615	-0.102
h	-5.019	-2.821	0.417	h	0.214	11.670	0.421	h	-4.970	-2.848	0.378
h	-11.291	-2.712	0.280	c	-1.412	9.007	-1.176	h	-11.209	-2.903	0.334
c	-8.149	-3.787	-0.803	h	-2.317	8.379	-1.249	c	-8.092	-3.868	-0.814
h	-7.282	-4.449	-0.639	h	-1.768	10.050	-1.123	h	-7.208	-4.514	-0.670
h	-9.045	-4.417	-0.671	c	-1.738	8.910	1.326	h	-8.973	-4.519	-0.676
c	-8.176	-3.455	1.703	h	-2.078	9.958	1.263	c	-8.094	-3.556	1.697
h	-9.067	-4.107	1.716	h	-2.625	8.287	1.116	h	-8.973	-4.225	1.717
h	-7.303	-4.130	1.738	c	-1.239	8.620	2.743	h	-7.208	-4.215	1.718
c	-8.178	-2.562	2.945	h	-0.897	7.573	2.808	c	-8.100	-2.668	2.943

h	-7.290	-1.908	2.931	h	-0.359	9.248	2.962	h	-7.218	-2.006	2.929
h	-9.056	-1.894	2.919	c	-2.317	8.867	3.804	h	-8.984	-2.008	2.921
c	-8.192	-3.368	4.248	h	-3.201	8.243	3.578	c	-8.107	-3.476	4.244
h	-7.315	-4.040	4.272	h	-2.660	9.915	3.741	h	-7.223	-4.140	4.268
h	-9.080	-4.027	4.262	c	-1.849	8.575	5.233	h	-8.989	-4.143	4.257
c	-8.192	-2.496	5.507	h	-1.502	7.528	5.297	c	-8.116	-2.605	5.503
h	-7.307	-1.835	5.492	h	-0.968	9.201	5.464	h	-7.234	-1.939	5.493
h	-9.071	-1.827	5.487	c	-2.930	8.813	6.292	h	-8.999	-1.941	5.480
c	-8.200	-3.300	6.810	h	-3.808	8.187	6.059	c	-8.125	-3.409	6.807
h	-7.322	-3.969	6.828	h	-3.276	9.859	6.227	h	-7.243	-4.073	6.829
h	-9.085	-3.960	6.823	c	-2.455	8.520	7.717	h	-9.006	-4.074	6.816
c	-8.200	-2.422	8.063	h	-3.252	8.698	8.454	c	-8.135	-2.530	8.059
h	-8.205	-3.026	8.981	h	-2.134	7.472	7.821	h	-8.142	-3.134	8.978
h	-7.309	-1.775	8.095	h	-1.599	9.156	7.990	h	-7.247	-1.878	8.095
h	-9.085	-1.767	8.090	c	-0.562	8.822	-2.436	h	-9.023	-1.880	8.081
c	-8.112	-3.244	-2.234	h	0.343	9.448	-2.367	c	-8.088	-3.308	-2.239
h	-8.980	-2.584	-2.401	h	-0.212	7.777	-2.495	h	-8.971	-2.663	-2.384
h	-7.216	-2.616	-2.367	c	-1.327	9.174	-3.716	h	-7.206	-2.660	-2.378
c	-8.111	-4.357	-3.287	h	-2.239	8.554	-3.779	c	-8.084	-4.405	-3.308
h	-7.246	-5.022	-3.115	h	-1.675	10.221	-3.658	h	-7.203	-5.056	-3.162
h	-9.010	-4.987	-3.155	c	-0.502	8.988	-4.993	h	-8.967	-5.054	-3.172
c	-8.068	-3.835	-4.726	h	-0.155	7.941	-5.054	c	-8.074	-3.858	-4.739
h	-7.171	-3.205	-4.858	h	0.410	9.607	-4.933	h	-7.191	-3.208	-4.875
h	-8.933	-3.171	-4.900	c	-1.266	9.340	-6.274	h	-8.955	-3.208	-4.886
c	-8.063	-4.945	-5.783	h	-2.179	8.722	-6.332	c	-8.067	-4.948	-5.815
h	-7.199	-5.608	-5.607	h	-1.612	10.387	-6.212	h	-7.188	-5.599	-5.666
h	-8.961	-5.574	-5.651	c	-0.436	9.149	-7.545	h	-8.950	-5.596	-5.681
c	-8.017	-4.413	-7.217	h	-0.106	8.105	-7.651	c	-8.054	-4.389	-7.240
h	-7.112	-3.809	-7.388	h	-1.011	9.410	-8.446	h	-7.164	-3.765	-7.414
h	-8.015	-5.232	-7.952	h	0.465	9.781	-7.530	h	-8.048	-5.194	-7.990
h	-8.887	-3.774	-7.433	c	-1.814	-8.584	0.430	h	-8.939	-3.763	-7.429
c	8.852	0.356	-0.199	c	-0.729	-9.422	0.733	c	8.853	0.448	-0.191
c	9.334	1.663	-0.373	c	0.552	-8.606	0.885	c	9.312	1.767	-0.346
c	8.176	2.650	-0.500	c	0.015	-7.202	0.626	c	8.140	2.738	-0.446

c	6.990	1.700	-0.360	c	-1.359	-7.236	0.367	c	6.970	1.767	-0.322
c	7.427	0.382	-0.188	c	0.545	-5.903	0.595	c	7.427	0.452	-0.175
c	5.593	1.818	-0.383	c	-0.414	-4.927	0.316	c	5.572	1.864	-0.346
c	4.940	0.593	-0.216	c	-2.464	-10.990	0.593	c	4.936	0.628	-0.203
c	11.347	0.475	-0.229	c	-1.094	-10.766	0.824	c	11.350	0.625	-0.244
c	10.728	1.728	-0.388	s	-2.020	-5.656	0.080	c	10.704	1.866	-0.375
s	6.107	-0.734	-0.029	s	-3.303	-9.451	0.253	s	6.122	-0.686	-0.039
s	10.123	-0.812	-0.053	h	-0.418	-11.591	1.051	s	10.151	-0.689	-0.078
h	11.317	2.637	-0.511	h	1.591	-5.651	0.775	h	11.250	2.802	-0.491
h	5.045	2.747	-0.536	c	1.157	-8.738	2.311	h	5.012	2.789	-0.483
c	8.198	3.721	0.626	h	1.504	-9.779	2.433	c	8.152	3.778	0.709
h	9.095	4.347	0.475	h	2.062	-8.107	2.349	h	9.034	4.425	0.567
h	7.331	4.386	0.471	c	1.633	-9.016	-0.154	h	7.270	4.430	0.581
c	8.177	3.369	-1.878	h	2.517	-8.378	0.016	c	8.126	3.490	-1.805
h	7.302	4.043	-1.902	h	1.950	-10.046	0.084	h	7.243	4.154	-1.810
h	9.067	4.023	-1.913	c	1.224	-8.935	-1.626	h	9.008	4.154	-1.829
c	8.158	2.466	-3.112	h	0.341	-9.573	-1.801	c	8.113	2.614	-3.059
h	9.038	1.801	-3.097	h	0.914	-7.904	-1.867	h	8.997	1.954	-3.057
h	7.272	1.810	-3.076	c	2.354	-9.358	-2.570	h	7.231	1.952	-3.038
c	8.145	3.260	-4.423	h	2.662	-10.392	-2.331	c	8.099	3.435	-4.353
h	9.030	3.922	-4.459	h	3.241	-8.726	-2.385	h	8.982	4.100	-4.375
h	7.265	3.929	-4.437	c	1.979	-9.275	-4.052	h	7.216	4.100	-4.355
c	8.126	2.377	-5.673	h	1.093	-9.908	-4.242	c	8.085	2.575	-5.620
h	9.008	1.711	-5.663	h	1.671	-8.242	-4.294	h	8.968	1.910	-5.618
h	7.243	1.713	-5.636	c	3.111	-9.697	-4.995	h	7.204	1.909	-5.599
c	8.107	3.168	-6.984	h	3.415	-10.731	-4.754	c	8.071	3.390	-6.916
h	8.989	3.832	-7.019	h	3.996	-9.067	-4.802	h	8.952	4.055	-6.936
h	7.226	3.833	-6.994	c	2.732	-9.608	-6.474	h	7.189	4.055	-6.916
c	8.089	2.277	-8.228	h	3.563	-9.918	-7.124	c	8.057	2.522	-8.175
h	8.076	2.873	-9.152	h	1.870	-10.253	-6.704	h	8.046	3.134	-9.089
h	8.977	1.626	-8.264	h	2.457	-8.578	-6.753	h	8.945	1.872	-8.221
h	7.201	1.626	-8.238	c	0.231	-8.370	3.474	h	7.169	1.871	-8.201
c	8.183	3.188	2.061	h	-0.115	-7.329	3.356	c	8.162	3.204	2.128
h	7.282	2.571	2.215	h	-0.671	-9.002	3.443	h	7.276	2.564	2.274

h	9.046	2.520	2.216	c	0.912	-8.525	4.838	h	9.040	2.549	2.254
c	8.215	4.309	3.106	h	1.263	-9.566	4.956	c	8.184	4.291	3.207
h	9.119	4.925	2.955	h	1.818	-7.893	4.869	h	9.070	4.935	3.061
h	7.356	4.985	2.944	c	0.006	-8.162	6.018	h	7.305	4.950	3.084
c	8.188	3.797	4.549	h	-0.900	-8.794	5.991	c	8.199	3.732	4.633
h	9.045	3.120	4.712	h	-0.347	-7.122	5.902	h	9.077	3.073	4.757
h	7.283	3.183	4.702	c	0.685	-8.314	7.383	h	7.313	3.088	4.782
c	8.222	4.913	5.598	h	1.036	-9.354	7.499	c	8.224	4.812	5.719
h	9.128	5.525	5.446	h	1.590	-7.683	7.409	h	9.109	5.455	5.569
h	7.367	5.591	5.433	c	-0.228	-7.949	8.556	h	7.346	5.469	5.597
c	8.192	4.392	7.036	h	-1.125	-8.587	8.575	c	8.242	4.240	7.139
h	9.054	3.739	7.241	h	0.287	-8.068	9.521	h	9.127	3.606	7.301
h	8.219	5.216	7.765	h	-0.567	-6.904	8.486	h	8.261	5.038	7.896
h	7.280	3.806	7.228	c	3.678	-0.643	-0.262	h	7.352	3.621	7.329
c	0.884	-3.706	0.167	h	3.327	-0.767	-1.300	c	0.866	-3.694	0.199
h	1.071	-3.361	1.196	h	3.700	-1.638	0.217	h	0.998	-3.338	1.233
h	1.841	-3.688	-0.384	c	5.082	-0.034	-0.227	h	1.850	-3.683	-0.300
c	0.306	-5.120	0.158	h	4.970	1.052	-0.404	c	0.284	-5.107	0.173
h	-0.652	-5.076	0.707	c	5.797	-0.240	1.121	h	-0.704	-5.052	0.665
c	-0.011	-5.615	-1.270	h	5.909	-1.327	1.293	c	0.047	-5.617	-1.265
h	-0.534	-6.582	-1.179	h	6.822	0.154	1.018	h	-0.488	-6.580	-1.193
h	-0.729	-4.918	-1.729	c	5.139	0.407	2.343	h	-0.639	-4.921	-1.773
c	1.195	-5.781	-2.199	h	4.142	-0.007	2.545	c	1.303	-5.802	-2.120
h	1.925	-6.504	-1.806	h	5.758	0.256	3.239	h	2.003	-6.526	-1.678
h	0.872	-6.146	-3.185	h	5.018	1.492	2.199	h	1.035	-6.176	-3.119
h	1.721	-4.828	-2.365	c	5.920	-0.627	-1.381	h	1.845	-4.856	-2.266
c	1.238	-6.084	0.921	h	5.803	-1.726	-1.391	c	1.165	-6.065	1.001
h	2.266	-6.003	0.526	h	6.986	-0.445	-1.164	h	2.216	-5.989	0.670
h	0.913	-7.115	0.699	c	5.604	-0.063	-2.771	h	0.853	-7.098	0.767
c	1.265	-5.898	2.443	h	4.535	-0.205	-3.010	c	1.098	-5.867	2.520
h	1.636	-4.891	2.702	h	5.769	1.029	-2.762	h	1.455	-4.859	2.794
h	0.233	-5.953	2.835	c	6.447	-0.692	-3.886	h	0.042	-5.915	2.845
c	2.132	-6.938	3.161	h	6.271	-1.781	-3.902	c	1.912	-6.905	3.300
h	3.161	-6.887	2.765	h	7.517	-0.560	-3.648	h	2.964	-6.861	2.971

h	1.762	-7.948	2.915	c	6.153	-0.104	-5.267	h	1.554	-7.915	3.037
c	2.158	-6.757	4.680	h	6.773	-0.574	-6.046	c	1.841	-6.713	4.816
h	2.786	-7.518	5.166	h	5.099	-0.252	-5.547	h	2.431	-7.473	5.347
h	2.559	-5.769	4.956	h	6.354	0.978	-5.291	h	2.226	-5.725	5.111
h	1.147	-6.835	5.109	c	-3.114	-12.245	0.628	h	0.803	-6.784	5.178
c	-0.877	3.640	-0.204	c	2.924	12.295	0.810	c	-0.895	3.644	-0.290
h	-1.805	3.609	0.389	h	-2.469	-13.100	0.862	h	-1.802	3.659	0.336
h	-1.106	3.312	-1.233	h	2.258	13.166	0.772	h	-1.166	3.271	-1.293
c	-0.303	5.056	-0.208	c	4.243	12.619	0.991	c	-0.292	5.044	-0.387
h	0.101	5.241	0.805	c	4.663	14.023	1.123	h	0.158	5.269	0.599
c	0.849	5.182	-1.221	n	6.067	14.095	1.311	c	0.822	5.089	-1.450
h	1.467	4.271	-1.164	c	6.766	12.915	1.327	h	1.421	4.168	-1.370
h	0.423	5.203	-2.240	c	-4.424	-12.586	0.419	h	0.355	5.068	-2.451
c	1.744	6.406	-1.006	c	-4.864	-13.987	0.523	c	1.752	6.300	-1.336
h	2.218	6.377	-0.013	n	-6.258	-14.079	0.277	h	2.267	6.311	-0.363
h	2.545	6.447	-1.759	c	-6.929	-12.918	-0.012	h	2.522	6.282	-2.121
h	1.182	7.349	-1.078	c	-6.916	-15.391	0.305	h	1.210	7.252	-1.434
c	-1.431	6.075	-0.472	h	-7.941	-15.222	0.661	c	-1.405	6.076	-0.660
h	-0.978	7.028	-0.791	h	-6.362	-15.990	1.039	h	-0.945	6.997	-1.053
h	-2.033	5.730	-1.334	c	-6.916	-16.070	-1.063	h	-2.055	5.699	-1.471
c	-2.353	6.352	0.721	h	-7.412	-17.048	-0.987	c	-2.262	6.446	0.557
h	-2.812	5.415	1.080	h	-7.463	-15.466	-1.800	h	-2.726	5.543	0.990
h	-1.747	6.733	1.563	h	-5.890	-16.234	-1.419	h	-1.607	6.857	1.346
c	-3.466	7.356	0.405	c	6.718	15.404	1.449	c	-3.364	7.461	0.235
h	-4.072	6.972	-0.434	h	7.580	15.259	2.114	h	-4.020	7.047	-0.550
h	-3.014	8.297	0.047	h	5.981	16.058	1.934	h	-2.905	8.366	-0.200
c	-4.374	7.646	1.602	c	7.154	15.981	0.104	c	-4.203	7.847	1.454
h	-5.163	8.368	1.345	h	7.628	16.960	0.261	h	-4.985	8.575	1.192
h	-4.867	6.728	1.960	h	7.883	15.322	-0.386	h	-4.701	6.967	1.890
h	-3.802	8.064	2.445	h	6.291	16.123	-0.561	h	-3.579	8.297	2.242
c	12.742	0.243	-0.205	s	-5.790	-11.539	0.017	c	12.724	0.281	-0.227
c	-12.709	-0.316	-0.051	s	5.640	11.544	1.104	c	-12.697	-0.397	0.012
h	13.366	1.138	-0.310	s	-8.542	-12.732	-0.341	h	12.978	-0.779	-0.114
h	-13.337	-1.210	0.048	s	8.398	12.702	1.525	h	-12.958	0.659	-0.125

c	-13.424	0.842	-0.210	o	3.945	15.017	1.089	c	-13.792	-1.217	0.112
c	-14.895	0.820	-0.235	o	-4.169	-14.963	0.786	c	-15.156	-0.672	0.026
n	-15.397	2.138	-0.391	o	-2.822	-0.186	-0.225	n	-16.107	-1.720	0.143
c	-14.485	3.156	-0.501	c	-3.536	0.610	-1.202	c	-15.630	-2.994	0.316
c	13.462	-0.916	-0.077	h	-2.926	0.664	-2.118	c	13.823	1.093	-0.333
c	14.933	-0.891	-0.080	h	-3.683	1.638	-0.824	c	15.184	0.535	-0.298
n	15.442	-2.207	0.070	c	-4.898	-0.028	-1.488	n	16.141	1.574	-0.444
c	14.534	-3.229	0.179	h	-4.738	-1.121	-1.549	c	15.671	2.856	-0.574
c	16.893	-2.430	0.073	c	-5.941	0.255	-0.390	c	17.573	1.254	-0.418
h	17.078	-3.290	0.731	c	-5.413	0.459	-2.860	h	18.070	1.975	-1.081
h	17.336	-1.526	0.511	h	-6.096	1.348	-0.332	h	17.663	0.242	-0.837
c	17.446	-2.682	-1.327	h	-6.904	-0.165	-0.729	c	18.157	1.313	0.991
h	18.533	-2.834	-1.271	c	-5.625	-0.295	1.003	h	19.226	1.061	0.956
h	16.997	-3.583	-1.769	h	-5.327	1.560	-2.913	h	18.058	2.322	1.414
h	17.255	-1.824	-1.985	h	-6.494	0.244	-2.919	h	17.658	0.593	1.654
c	-16.846	2.360	-0.466	c	-4.726	-0.170	-4.077	c	-17.542	-1.409	0.102
h	-17.037	3.347	-0.023	h	-4.716	0.151	1.427	h	-18.038	-2.270	-0.366
h	-17.303	1.579	0.158	h	-6.457	-0.095	1.694	h	-17.640	-0.527	-0.544
c	-17.373	2.289	-1.897	h	-5.469	-1.384	0.972	c	-18.117	-1.133	1.489
h	-18.460	2.451	-1.897	h	-3.638	0.021	-4.048	h	-19.188	-0.899	1.403
h	-16.912	3.066	-2.522	h	-4.842	-1.267	-4.029	h	-18.012	-2.013	2.139
h	-17.174	1.304	-2.340	c	-5.279	0.338	-5.413	h	-17.617	-0.275	1.958
s	12.872	-2.571	0.106	h	-5.162	1.434	-5.461	s	13.884	2.847	-0.528
s	-12.826	2.493	-0.398	h	-6.365	0.147	-5.450	s	-13.843	-2.966	0.338
s	14.843	-4.847	0.361	c	-4.604	-0.303	-6.627	s	16.550	4.249	-0.757
s	-14.786	4.775	-0.693	h	-5.023	0.078	-7.570	s	-16.502	-4.394	0.479
o	-15.623	-0.162	-0.135	h	-3.522	-0.098	-6.636	o	-15.476	0.502	-0.127
o	15.657	0.094	-0.189	h	-4.733	-1.397	-6.623	o	15.498	-0.644	-0.170

Table S3. Cartesian coordinates of **BDT(CDTRH)$_2$** isomers 4,5 and 6, optimized at the DFT/PBE/TZVP level of theory (units in Ångströms).

isomer 4				**isomer 5**				**isomer 6**			
atom	**x**	**y**	**z**	**atom**	**x**	**y**	**z**	**atom**	**x**	**y**	**z**

c	-0.679	-1.234	0.057	c	-0.639	-1.233	0.242	c	-0.628	-1.506	0.305
c	0.744	-1.178	0.202	c	0.785	-1.145	0.368	c	0.788	-1.389	0.418
c	1.432	0.037	0.233	c	1.443	0.087	0.375	c	1.437	-0.162	0.465
c	0.659	1.222	0.155	c	0.636	1.252	0.307	c	0.637	1.000	0.413
c	-0.766	1.165	0.029	c	-0.790	1.163	0.210	c	-0.790	0.898	0.290
c	-1.449	-0.050	-0.043	c	-1.444	-0.069	0.151	c	-1.439	-0.342	0.251
c	-1.181	-2.566	0.079	c	-1.114	-2.573	0.260	c	-1.057	-2.863	0.305
c	-0.214	-3.532	0.251	c	-0.125	-3.522	0.411	c	-0.025	-3.775	0.404
h	-2.243	-2.789	-0.006	h	-2.172	-2.813	0.177	h	-2.105	-3.151	0.262
c	1.151	2.555	0.225	c	1.105	2.594	0.340	c	1.089	2.349	0.474
c	0.170	3.523	0.184	c	0.105	3.543	0.306	c	0.087	3.286	0.358
h	2.213	2.780	0.315	h	2.164	2.839	0.384	h	2.131	2.615	0.647
o	2.781	0.200	0.414	o	2.786	0.312	0.508	o	2.805	-0.091	0.619
s	1.409	-2.807	0.382	s	1.479	-2.768	0.538	o	-2.780	-0.571	0.116
s	-1.450	2.797	0.042	s	-1.502	2.786	0.227	s	1.560	-2.969	0.503
c	1.171	7.283	0.412	c	-0.170	7.431	0.217	s	-1.504	2.519	0.169
c	-0.215	7.228	0.234	c	1.160	7.110	0.511	c	-0.135	7.169	0.610
c	-0.813	8.631	0.193	c	1.995	8.376	0.684	c	1.170	6.847	0.217
c	0.449	9.470	0.370	c	0.930	9.443	0.444	c	1.996	8.115	-0.010
c	1.580	8.646	0.495	c	-0.314	8.847	0.178	c	0.954	9.183	0.332
c	0.749	10.831	0.437	c	0.877	10.837	0.414	c	-0.269	8.584	0.678
c	2.120	11.087	0.616	c	-0.404	11.342	0.127	c	0.914	10.576	0.439
c	0.298	4.949	0.237	c	0.239	4.971	0.335	c	-0.336	11.073	0.846
c	-0.704	5.917	0.135	c	1.388	5.728	0.583	c	0.222	4.716	0.361
s	3.036	9.555	0.700	s	-1.566	10.008	-0.111	c	1.361	5.464	0.060
s	1.894	5.703	0.466	s	-1.159	6.020	0.007	s	-1.486	9.736	1.116
h	-1.751	5.652	-0.009	h	2.346	5.265	0.819	s	-1.131	5.765	0.833
h	0.011	11.629	0.359	h	1.721	11.506	0.589	h	2.278	4.992	-0.289
c	-1.515	8.923	-1.163	c	2.610	8.474	2.108	h	1.747	11.251	0.241
h	-2.404	8.272	-1.226	h	3.344	7.655	2.210	c	3.191	8.228	0.981
h	-1.895	9.959	-1.125	h	3.191	9.412	2.158	h	3.613	9.243	0.891
c	-1.828	8.863	1.347	c	3.143	8.462	-0.361	h	2.785	8.159	2.005
h	-2.189	9.903	1.268	h	3.676	9.414	-0.193	c	2.431	8.170	-1.503
h	-2.705	8.219	1.155	h	3.866	7.661	-0.130	h	3.003	7.253	-1.723

c	-1.308	8.608	2.763	c	2.726	8.365	-1.831	h	1.519	8.112	-2.119
h	-0.958	7.565	2.846	h	2.217	7.403	-2.008	c	3.256	9.385	-1.931
h	-0.429	9.246	2.954	h	1.988	9.152	-2.059	h	2.678	10.309	-1.761
c	-2.369	8.873	3.837	c	3.915	8.494	-2.789	h	4.165	9.466	-1.311
h	-3.254	8.240	3.643	h	4.662	7.715	-2.553	c	3.669	9.319	-3.406
h	-2.718	9.918	3.756	h	4.421	9.461	-2.616	h	2.764	9.245	-4.035
c	-1.870	8.617	5.262	c	3.525	8.388	-4.266	h	4.238	8.388	-3.582
h	-1.520	7.572	5.344	h	3.028	7.417	-4.443	c	4.507	10.516	-3.862
h	-0.986	9.250	5.458	h	2.771	9.161	-4.500	h	3.936	11.448	-3.696
c	-2.927	8.881	6.339	c	4.709	8.532	-5.227	h	5.408	10.594	-3.227
h	-3.810	8.248	6.142	h	5.463	7.762	-4.990	c	4.934	10.443	-5.331
h	-3.276	9.924	6.256	h	5.202	9.504	-5.051	h	4.035	10.365	-5.966
c	-2.419	8.622	7.759	c	4.309	8.420	-6.699	h	5.504	9.512	-5.496
h	-3.199	8.820	8.510	h	5.178	8.530	-7.364	c	5.773	11.643	-5.777
h	-2.095	7.577	7.882	h	3.847	7.444	-6.913	h	6.065	11.561	-6.834
h	-1.558	9.266	7.997	h	3.579	9.198	-6.973	h	5.215	12.585	-5.658
c	-0.656	8.740	-2.417	c	1.624	8.422	3.277	h	6.695	11.726	-5.182
h	0.240	9.380	-2.347	h	0.906	9.255	3.192	c	4.312	7.200	0.810
h	-0.291	7.701	-2.466	h	1.031	7.494	3.219	h	3.907	6.183	0.941
c	-1.413	9.075	-3.706	c	2.326	8.491	4.638	h	4.716	7.244	-0.216
h	-2.315	8.440	-3.777	h	3.038	7.650	4.724	c	5.460	7.409	1.804
h	-1.778	10.117	-3.657	h	2.935	9.412	4.690	h	5.872	8.427	1.679
c	-0.569	8.896	-4.972	c	1.363	8.457	5.827	h	5.063	7.366	2.834
h	-0.208	7.853	-5.025	h	0.746	7.543	5.772	c	6.588	6.385	1.651
h	0.335	9.526	-4.899	h	0.657	9.304	5.750	h	6.980	6.424	0.618
c	-1.318	9.237	-6.264	c	2.066	8.510	7.187	h	6.177	5.367	1.781
h	-2.222	8.608	-6.336	h	2.767	7.660	7.265	c	7.745	6.590	2.634
h	-1.677	10.280	-6.210	h	2.688	9.421	7.239	h	8.156	7.606	2.502
c	-0.465	9.055	-7.522	c	1.098	8.484	8.371	h	7.354	6.553	3.665
h	-0.121	8.014	-7.621	h	0.486	7.568	8.364	c	8.864	5.559	2.472
h	-1.029	9.308	-8.432	h	1.632	8.519	9.332	h	9.296	5.596	1.460
h	0.428	9.697	-7.493	h	0.409	9.342	8.341	h	9.680	5.733	3.189
c	-1.672	-8.649	0.383	c	0.247	-8.822	0.736	h	8.489	4.537	2.635
c	-0.580	-9.455	0.744	c	-1.017	-9.412	0.568	c	0.408	-9.045	0.977

c	0.668	-8.607	0.965	c	-2.084	-8.340	0.356	c	-0.755	-9.690	0.522
c	0.106	-7.218	0.681	c	-1.226	-7.080	0.430	c	-1.771	-8.666	0.011
c	-1.250	-7.287	0.349	c	0.117	-7.407	0.652	c	-1.000	-7.368	0.266
c	0.607	-5.908	0.675	c	-1.444	-5.700	0.323	c	0.256	-7.639	0.823
c	-0.358	-4.955	0.340	c	-0.273	-4.948	0.463	c	-1.204	-5.998	0.032
c	-2.237	-11.085	0.489	c	0.314	-11.317	0.857	c	-0.126	-5.207	0.434
c	-0.894	-10.814	0.804	c	-0.977	-10.804	0.636	c	0.490	-11.519	1.299
s	-1.930	-5.722	0.016	s	1.132	-6.002	0.737	c	-0.708	-11.073	0.714
s	-3.109	-9.572	0.111	s	1.503	-9.991	0.982	s	1.186	-6.201	1.101
h	-0.184	-11.598	1.064	h	-1.837	-11.468	0.533	s	1.580	-10.144	1.624
h	1.634	-5.631	0.915	h	-2.413	-5.234	0.144	h	-1.502	-11.775	0.460
c	1.196	-8.729	2.422	c	-2.785	-8.479	-1.024	h	-2.087	-5.565	-0.437
h	1.559	-9.763	2.561	h	-3.377	-9.412	-1.007	c	-2.036	-8.804	-1.516
h	2.083	-8.079	2.512	h	-3.516	-7.656	-1.110	h	-2.613	-7.922	-1.841
c	1.807	-8.987	-0.020	c	-3.166	-8.372	1.471	h	-1.064	-8.736	-2.032
h	2.667	-8.326	0.191	h	-3.893	-7.570	1.253	c	-3.064	-8.761	0.870
h	2.138	-10.009	0.232	h	-3.720	-9.322	1.372	h	-3.450	-9.792	0.793
c	1.461	-8.915	-1.508	c	-2.661	-8.223	2.908	h	-2.775	-8.626	1.925
h	0.591	-9.561	-1.716	h	-1.924	-9.014	3.125	c	-4.186	-7.780	0.522
h	1.153	-7.889	-1.768	h	-2.128	-7.264	3.015	h	-3.817	-6.745	0.614
c	2.628	-9.337	-2.406	c	-3.795	-8.290	3.938	h	-4.492	-7.910	-0.530
h	2.936	-10.366	-2.147	h	-4.321	-9.257	3.840	c	-5.415	-7.948	1.423
h	3.503	-8.696	-2.196	h	-4.544	-7.511	3.709	h	-5.114	-7.817	2.478
c	2.302	-9.272	-3.901	c	-3.319	-8.120	5.384	h	-5.790	-8.985	1.342
h	1.424	-9.909	-4.111	h	-2.562	-8.891	5.612	c	-6.548	-6.973	1.094
h	2.000	-8.242	-4.164	h	-2.802	-7.149	5.485	h	-6.170	-5.937	1.168
c	3.463	-9.702	-4.803	c	-4.448	-8.201	6.416	h	-6.853	-7.109	0.040
h	3.763	-10.731	-4.540	h	-4.958	-9.175	6.318	c	-7.776	-7.125	1.997
h	4.341	-9.067	-4.591	h	-5.207	-7.436	6.182	h	-7.470	-6.987	3.049
c	3.128	-9.631	-6.294	c	-3.965	-8.019	7.856	h	-8.154	-8.159	1.924
h	3.979	-9.948	-6.915	h	-4.797	-8.085	8.573	c	-8.899	-6.144	1.657
h	2.275	-10.282	-6.541	h	-3.228	-8.790	8.129	h	-9.766	-6.274	2.322
h	2.860	-8.607	-6.594	h	-3.483	-7.039	7.993	h	-8.559	-5.101	1.754
c	0.196	-8.386	3.529	c	-1.872	-8.477	-2.251	h	-9.250	-6.282	0.623

h	-0.157	-7.349	3.400	h	-1.266	-7.555	-2.259	c	-2.763	-10.072	-1.971
h	-0.695	-9.030	3.435	h	-1.160	-9.316	-2.184	h	-2.171	-10.961	-1.694
c	0.788	-8.549	4.933	c	-2.655	-8.578	-3.565	h	-3.730	-10.165	-1.449
h	1.141	-9.588	5.064	h	-3.273	-9.494	-3.555	c	-3.012	-10.091	-3.484
h	1.683	-7.909	5.031	h	-3.366	-7.733	-3.632	h	-3.603	-9.202	-3.767
c	-0.201	-8.209	6.053	c	-1.765	-8.585	-4.810	h	-2.047	-9.996	-4.013
h	-1.098	-8.847	5.953	h	-1.063	-9.436	-4.752	c	-3.733	-11.352	-3.969
h	-0.553	-7.169	5.925	h	-1.138	-7.675	-4.816	h	-4.694	-11.453	-3.432
c	0.380	-8.376	7.460	c	-2.548	-8.666	-6.124	h	-3.138	-12.241	-3.697
h	0.730	-9.415	7.586	h	-3.177	-9.573	-6.116	c	-3.998	-11.366	-5.478
h	1.277	-7.740	7.559	h	-3.247	-7.813	-6.182	h	-4.594	-10.477	-5.749
c	-0.616	-8.033	8.569	c	-1.652	-8.676	-7.364	h	-3.039	-11.264	-6.014
h	-1.509	-8.676	8.515	h	-0.967	-9.538	-7.353	c	-4.719	-12.629	-5.953
h	-0.172	-8.164	9.567	h	-2.243	-8.732	-8.290	h	-5.696	-12.739	-5.458
h	-0.956	-6.989	8.490	h	-1.035	-7.765	-7.416	h	-4.895	-12.610	-7.038
c	3.677	-0.617	-0.379	c	3.719	-0.643	-0.047	h	-4.130	-13.532	-5.727
h	3.286	-0.658	-1.409	h	3.347	-0.965	-1.033	c	3.535	0.186	-0.607
h	3.710	-1.648	0.018	h	3.787	-1.530	0.608	h	3.162	1.127	-1.046
c	5.085	-0.020	-0.350	c	5.105	-0.005	-0.174	h	3.345	-0.624	-1.333
h	4.976	1.077	-0.436	h	4.966	0.994	-0.627	c	5.021	0.292	-0.275
c	5.851	-0.339	0.949	c	5.826	0.161	1.178	h	5.102	1.006	0.566
h	5.963	-1.436	1.025	h	5.916	-0.834	1.650	c	5.611	-1.046	0.217
h	6.874	0.059	0.838	h	6.858	0.485	0.964	h	6.634	-0.848	0.581
c	5.244	0.206	2.244	c	5.199	1.146	2.169	h	5.033	-1.379	1.094
h	4.253	-0.222	2.450	h	4.203	0.825	2.499	c	5.657	-2.171	-0.821
h	5.897	-0.020	3.100	h	5.836	1.252	3.060	h	6.260	-1.897	-1.699
h	5.121	1.299	2.196	h	5.090	2.144	1.717	h	6.105	-3.077	-0.386
c	5.875	-0.525	-1.578	c	5.963	-0.856	-1.137	h	4.654	-2.449	-1.176
h	5.754	-1.621	-1.664	h	5.922	-1.915	-0.822	c	5.796	0.888	-1.468
h	6.949	-0.360	-1.390	h	7.016	-0.551	-1.014	h	5.489	0.391	-2.405
c	5.505	0.138	-2.910	c	5.597	-0.748	-2.622	h	6.866	0.650	-1.341
h	4.428	0.014	-3.116	h	4.552	-1.061	-2.789	c	5.649	2.407	-1.626
h	5.676	1.226	-2.830	h	5.649	0.312	-2.930	h	4.584	2.676	-1.741
c	6.301	-0.411	-4.099	c	6.510	-1.581	-3.528	h	5.990	2.899	-0.698

h	6.123	-1.498	-4.183	h	6.458	-2.639	-3.218	c	6.430	2.979	-2.814
h	7.380	-0.295	-3.898	h	7.557	-1.270	-3.371	h	6.083	2.495	-3.743
c	5.951	0.268	-5.424	c	6.157	-1.464	-5.012	h	7.495	2.709	-2.709
h	6.537	-0.146	-6.258	h	6.829	-2.071	-5.635	c	6.297	4.497	-2.947
h	4.886	0.139	-5.669	h	5.127	-1.803	-5.204	h	6.868	4.880	-3.805
h	6.152	1.350	-5.382	h	6.232	-0.421	-5.358	h	5.246	4.794	-3.088
c	-2.957	-12.304	0.426	c	0.653	-12.685	0.966	h	6.669	5.008	-2.044
c	2.842	12.301	0.726	c	-0.753	12.710	0.034	c	-3.725	0.362	0.690
h	-4.014	-12.254	0.141	h	-0.185	-13.384	0.857	h	-3.804	1.250	0.043
h	3.928	12.233	0.857	h	0.069	13.415	0.199	h	-3.370	0.680	1.686
c	2.382	13.591	0.692	c	-1.954	13.317	-0.228	c	-5.081	-0.333	0.805
c	3.309	14.728	0.819	c	-2.061	14.783	-0.276	h	-5.287	-0.801	-0.176
n	2.592	15.951	0.738	n	-3.396	15.163	-0.573	c	-5.041	-1.442	1.873
c	1.233	15.882	0.577	c	-4.316	14.162	-0.748	h	-4.086	-1.983	1.783
c	-2.523	-13.580	0.674	c	1.857	-13.301	1.187	h	-5.036	-0.970	2.872
c	-3.435	-14.728	0.545	c	1.950	-14.768	1.256	c	-6.191	-2.447	1.780
n	-2.746	-15.933	0.845	n	3.294	-15.159	1.484	h	-6.187	-2.962	0.807
c	-1.424	-15.839	1.195	c	4.232	-14.166	1.605	h	-6.110	-3.214	2.564
c	-3.466	-17.212	0.802	c	3.625	-16.584	1.612	h	-7.175	-1.967	1.895
h	-2.738	-17.973	0.490	h	4.639	-16.710	1.212	c	-6.181	0.711	1.085
h	-4.237	-17.098	0.028	h	2.906	-17.118	0.977	h	-7.070	0.190	1.476
c	-4.094	-17.573	2.146	c	3.541	-17.072	3.056	h	-5.845	1.378	1.900
h	-4.624	-18.532	2.058	h	3.787	-18.143	3.097	c	-6.608	1.551	-0.124
h	-3.324	-17.679	2.922	h	4.255	-16.533	3.694	h	-5.739	2.082	-0.552
h	-4.820	-16.810	2.457	h	2.527	-16.940	3.457	h	-6.972	0.878	-0.920
c	3.313	17.225	0.860	c	-3.747	16.586	-0.647	c	-7.697	2.577	0.207
h	2.776	17.952	0.237	h	-4.549	16.675	-1.393	h	-7.331	3.251	1.001
h	4.313	17.047	0.442	h	-2.847	17.101	-1.008	h	-8.570	2.053	0.633
c	3.407	17.705	2.307	c	-4.190	17.147	0.702	c	-8.136	3.403	-1.004
h	3.962	18.653	2.343	h	-4.436	18.213	0.595	h	-8.918	4.129	-0.736
h	2.407	17.877	2.727	h	-5.085	16.625	1.068	h	-7.291	3.967	-1.429
h	3.939	16.973	2.929	h	-3.388	17.054	1.447	h	-8.538	2.759	-1.801
s	-0.916	-14.125	1.162	s	3.448	-12.569	1.421	c	0.810	-12.863	1.603
s	0.725	14.169	0.500	s	-3.523	12.571	-0.549	c	-0.668	12.437	1.018

s	-0.385	-17.067	1.594	s	5.859	-14.333	1.873	h	0.038	-13.597	1.346
s	0.156	17.136	0.455	s	-5.929	14.314	-1.099	h	0.144	13.146	0.817
o	4.525	14.678	0.969	o	-1.162	15.598	-0.097	c	-1.839	13.037	1.397
o	-4.618	-14.701	0.224	o	1.033	-15.574	1.136	c	-1.936	14.502	1.505
o	-2.808	-0.213	-0.119	o	-2.794	-0.287	0.086	n	-3.247	14.876	1.895
c	-3.540	0.593	-1.075	c	-3.611	0.618	-0.693	c	-4.156	13.871	2.109
h	-2.942	0.662	-1.998	h	-3.071	0.867	-1.620	c	1.923	-13.416	2.179
h	-3.685	1.616	-0.681	h	-3.785	1.553	-0.129	c	2.008	-14.867	2.412
c	-4.904	-0.043	-1.353	c	-4.958	-0.037	-1.007	n	3.248	-15.189	3.021
h	-4.742	-1.133	-1.445	h	-4.752	-1.073	-1.335	c	4.112	-14.157	3.286
c	-5.929	0.209	-0.230	c	-5.909	-0.083	0.204	c	3.544	-16.583	3.373
c	-5.444	0.481	-2.701	c	-5.622	0.718	-2.181	h	4.631	-16.708	3.278
h	-6.080	1.300	-0.137	h	-6.079	0.952	0.553	h	3.033	-17.200	2.622
h	-6.897	-0.198	-0.566	h	-6.888	-0.441	-0.157	c	3.073	-16.939	4.781
c	-5.592	-0.383	1.141	c	-5.471	-0.957	1.383	h	3.311	-17.991	4.994
h	-5.364	1.584	-2.723	h	-5.614	1.802	-1.968	h	3.577	-16.316	5.531
h	-6.525	0.262	-2.747	h	-6.687	0.430	-2.214	h	1.986	-16.811	4.875
c	-4.776	-0.107	-3.948	c	-5.007	0.462	-3.561	c	-3.574	16.295	2.084
h	-4.677	0.050	1.566	h	-4.546	-0.593	1.847	h	-4.631	16.413	1.811
h	-6.415	-0.203	1.850	h	-6.254	-0.981	2.155	h	-2.944	16.846	1.374
h	-5.439	-1.471	1.076	h	-5.291	-1.994	1.059	c	-3.322	16.765	3.514
h	-3.689	0.090	-3.935	h	-3.939	0.742	-3.568	h	-3.574	17.831	3.601
h	-4.884	-1.207	-3.931	h	-5.038	-0.621	-3.776	h	-3.946	16.207	4.225
c	-5.357	0.435	-5.258	c	-5.719	1.220	-4.687	h	-2.265	16.641	3.787
h	-5.250	1.534	-5.274	h	-5.688	2.302	-4.471	s	3.390	-12.612	2.748
h	-6.443	0.237	-5.281	h	-6.787	0.943	-4.691	s	-3.384	12.285	1.808
c	-4.700	-0.162	-6.504	c	-5.116	0.957	-6.068	s	5.612	-14.243	3.985
h	-5.139	0.243	-7.426	h	-5.646	1.515	-6.853	s	-5.741	14.016	2.569
h	-3.620	0.053	-6.526	h	-4.057	1.258	-6.104	o	-1.046	15.320	1.294
h	-4.820	-1.257	-6.531	h	-5.165	-0.112	-6.327	o	1.162	-15.712	2.138