Supplementary Information

Exploration of Nonlinear Optical Properties for First Theoretical Framework of Non-Fullerene DTS(FBTTh$_2$)$_2$ Based Derivatives

Muhammad Usman Khan,*[1] Shabbir Hussain,[2] Muhammad Adnan Asghar,[3] Khurram Shahzad Munawar,[4] Rasheed Ahmad Khera,[5] Muhammad Imran[6], Mohamed M. Ibrahim,[7] Mahmoud M. Hessien,[7] Gaber A. M. Mersal,[7]

[1]*Department of Chemistry, University of Okara, Okara-56300, Pakistan*

[2]*Department of Chemistry, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, 64200, Pakistan*

[3]*Department of Chemistry, Division of Science and Technology, University of Education Lahore, Pakistan*

[4]*Department of Chemistry, University of Mianwali, Punjab, Pakistan*

[4]*Department of Chemistry, University of Agriculture, 38000, Faisalabad, Pakistan*

[6]*Department of Chemistry, Faculty of Science, King Khalid University, P.O. Box 9004, Abha 61413, Saudi Arabia.*

[7]*Department of Chemistry, College of Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia.*

*** Corresponding author E-mail address:**

Dr. Muhammad Usman Khan (usman.chemistry@gmail.com)

Table S1: Cartesian coordinates of **DTS(FBTTh$_2$)$_2$R1**

Atom	X-axis	Y-axis	Z-axis
C	-3.19877	0.798845	0.014766
C	-2.74975	2.110493	0.010289
C	-1.34948	2.243835	0.004107
C	-0.72095	1.005319	0.0027
C	1.349461	2.243858	-0.00384
C	0.720955	1.005331	-0.00251
C	2.749738	2.11054	-0.01005
C	3.198777	0.798899	-0.01461
S	1.827616	-0.3152	-0.01092
S	-1.82759	-0.31523	0.010994

C	4.933958	-1.00617	-0.04797
C	4.567131	0.32695	-0.02221
C	5.705731	1.209645	-0.00332
C	7.067046	0.705743	-0.0151
C	7.3584	-0.69871	-0.04658
C	6.243887	-1.5114	-0.05904
H	6.332095	-2.5937	-0.07771
H	3.447798	2.939688	-0.01093
N	7.986067	1.666618	0.007203
N	5.654231	2.540126	0.027986
C	9.051692	-2.57258	-0.12313
C	8.701764	-1.23847	-0.06359
C	11.17725	-1.64091	-0.07064
C	10.43735	-2.80121	-0.12739
H	8.320352	-3.37364	-0.17373
H	10.88788	-3.78798	-0.18981
S	10.1415	-0.24278	0.000212
C	12.61064	-1.49131	-0.06381
C	13.36524	-0.35982	-0.24791
C	14.76033	-0.59719	-0.17746
C	15.08468	-1.90357	0.057645
H	12.92498	0.614092	-0.44434
H	15.51507	0.174456	-0.30321
S	13.64746	-2.87487	0.208487
C	-6.2439	-1.51144	0.059003
C	-7.3584	-0.69874	0.046582
C	-7.06703	0.705708	0.01519
C	-5.70571	1.209595	0.003466
C	-4.56712	0.326889	0.022322
C	-4.93396	-1.00623	0.047986
H	-6.33212	-2.59375	0.077586
Si	-0.00002000	3.560186	0.000174
C	-0.00382	4.623334	-1.54352
H	-0.00522	4.002392	-2.44492
H	-0.88997	5.267232	-1.57211
H	0.881336	5.268444	-1.57565
C	0.003763	4.623252	1.543929
H	0.005176	4.002265	2.445296
H	0.889906	5.267164	1.572548
H	-0.8814	5.268346	1.576088
S	7.189942	3.087482	0.040751
H	-3.44783	2.939629	0.011223
S	-7.18989	3.087452	-0.04051

N	-5.65419	2.540076	-0.02776
N	-7.98604	1.666596	-0.00707
C	-10.4374	-2.80121	0.127257
C	-11.1773	-1.64091	0.070474
C	-8.70177	-1.23849	0.063532
C	-9.05171	-2.5726	0.123065
H	-10.8879	-3.78798	0.18967
H	-8.32038	-3.37366	0.173712
S	-10.1415	-0.24279	-0.00034
C	-15.0847	-1.90353	-0.05799
C	-14.7603	-0.59716	0.17714
C	-13.3652	-0.3598	0.247656
C	-12.6106	-1.49129	0.063575
H	-15.5151	0.174501	0.302864
H	-12.925	0.61411	0.444113
S	-13.6475	-2.87484	-0.20878
C	-16.4357	-2.51399	-0.18917
H	-17.2031	-1.74339	-0.06467
H	-16.5837	-2.97842	-1.17162
H	-16.6123	-3.28781	0.567527
C	16.43573	-2.51405	0.188759
H	17.20312	-1.74346	0.064251
H	16.58369	-2.97851	1.171184
H	16.61226	-3.28785	-0.56797
F	3.973719	-1.94169	-0.06414
F	-3.97373	-1.94176	0.064107

Table S2: Cartesian coordinates of **MSTD2**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-2.32592	2.05253	0.016087
C	-1.8385	3.350738	0.048113
C	-0.43529	3.444276	-0.00676
C	0.155487	2.191142	-0.08327
C	2.26525	3.370941	-0.12567
C	1.594939	2.155298	-0.14956
C	3.661448	3.185234	-0.20379
C	4.058061	1.866326	-0.28699
S	2.662146	0.800982	-0.26223
S	-0.98721	0.90277	-0.08516
C	5.653689	0.035031	-0.86733
C	5.405191	1.330525	-0.38743
C	6.513051	2.102321	-0.00201

C	7.800325	1.61033	-0.10881
C	8.045254	0.316096	-0.58874
C	6.939814	-0.46302	-0.9579
H	7.093624	-1.48171	-1.30725
H	4.381174	4.00013	-0.22965
C	9.84104	-1.24394	-1.50849
C	9.393157	-0.22019	-0.70602
C	11.84513	-0.7022	-0.4524
C	11.21644	-1.5159	-1.36596
H	9.193165	-1.76944	-2.20328
H	11.73673	-2.29333	-1.91965
S	10.70624	0.420401	0.249434
C	13.22684	-0.68887	-0.05208
C	13.8221	-0.00262	0.982998
C	15.20914	-0.23152	1.082043
C	15.69845	-1.09443	0.131359
H	13.26278	0.630128	1.666137
H	15.82946	0.197885	1.864076
S	14.4129	-1.62343	-0.92682
C	-5.43096	-0.17541	0.066451
C	-6.52578	0.671861	0.110489
C	-6.19084	2.069657	0.122425
C	-4.81592	2.535185	0.094714
C	-3.70663	1.61931	0.050054
C	-4.11315	0.294396	0.039378
H	-5.55035	-1.25443	0.048434
Si	0.94903800	4.718776	-0.01569
C	0.921778	5.840231	-1.51675
H	0.872149	5.253846	-2.43968
H	0.051059	6.504838	-1.49003
H	1.820319	6.466195	-1.55743
C	1.050995	5.719534	1.565487
H	1.078305	5.062842	2.440794
H	1.950395	6.345428	1.579125
H	0.181992	6.379579	1.664081
H	-2.5131	4.196844	0.108191
S	-6.24835	4.454514	0.157994
N	-4.72629	3.864607	0.112114
N	-7.08139	3.054407	0.158449
C	-9.64469	-1.34857	0.181125
C	-10.3637	-0.15978	0.178107
C	-7.87558	0.17948	0.139735
C	-8.26503	-1.15363	0.160573

H	-10.1209	-2.32428	0.213599
H	-7.55452	-1.97476	0.16895
S	-9.28856	1.216277	0.146855
C	-14.2628	-0.34104	0.205801
C	-13.8803	1.003167	0.297097
C	-12.504	1.194039	0.293669
C	-11.7751	0.013261	0.196663
H	-14.6236	1.789347	0.351769
H	-12.0299	2.168953	0.372245
S	-12.843	-1.36115	0.106826
F	-3.17672	-0.66484	-0.00344
C	17.06707	-1.55492	-0.04967
C	18.13062	-0.78095	0.445531
C	17.35115	-2.76299	-0.71161
C	19.41246	-1.26744	0.274403
H	17.93882	0.177036	0.922995
C	18.65479	-3.2162	-0.89327
H	16.52501	-3.37021	-1.07486
H	18.8379	-4.15299	-1.41437
C	19.70311	-2.47224	-0.38194
C	-17.8682	-0.7634	-0.56797
C	-17.5037	-2.10289	-0.40743
C	-18.4699	-3.08844	-0.5701
C	-19.7655	-2.69896	-0.91848
C	-20.1088	-1.36041	-1.08982
C	-19.1474	-0.3681	-0.90183
C	-15.5905	-0.82495	0.080187
H	-18.2425	-4.14308	-0.45666
H	-20.5226	-3.46692	-1.06028
H	-21.1272	-1.09348	-1.36191
H	-19.3747	0.691174	-0.99941
C	-16.6997	0.096991	-0.27609
O	-16.6899	1.314921	-0.34327
C	-16.0838	-2.14504	0.055438
C	-15.4455	-3.31223	0.494748
N	-15.805	-4.59464	-0.03505
O	-15.8127	-5.57309	0.699341
O	-16.1289	-4.62079	-1.22481
N	-14.4968	-3.33522	1.569404
O	-13.6703	-4.23929	1.605073
O	-14.5408	-2.41019	2.378824
H	4.82052	-0.59121	-1.18141
C	21.65764	-1.43331	0.32708

C	21.19277	-2.6218	-0.4374
C	21.97976	-3.7309	0.29062
H	22.05217	-4.65848	-0.28527
C	23.00824	-1.59509	0.917558
C	23.34023	-3.0574	0.530167
H	23.9419	-3.56222	1.290519
N	20.62517	-0.679	0.704663
C	20.67984	0.497626	1.545534
H	20.24819	1.355367	1.018356
H	20.11362	0.328117	2.467916
H	21.71933	0.722604	1.790843
H	23.7565	-0.87896	0.549568
H	22.96364	-1.46162	2.010377
H	23.92156	-3.06577	-0.40042
H	21.48358	-3.96019	1.243074
H	21.5536	-2.58387	-1.48365
H	6.355679	3.100669	0.399488
H	8.636399	2.246677	0.178173

Table S3: Cartesian coordinates of **MSTD3**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	1.220168	2.381066	-0.21223
C	0.730865	3.664134	-0.01744
C	-0.67268	3.761045	-0.05639
C	-1.26127	2.525491	-0.28512
C	-3.37373	3.695001	-0.16825
C	-2.70102	2.493518	-0.34557
C	-4.77038	3.514273	-0.24885
C	-5.16505	2.212808	-0.48226
S	-3.76609	1.158021	-0.60461
S	-0.1164	1.250506	-0.45502
C	-6.76383	0.447409	-1.23304
C	-6.51188	1.684492	-0.61908
C	-7.61544	2.402004	-0.13024
C	-8.90194	1.914042	-0.26177
C	-9.14967	0.676502	-0.87212
C	-8.04865	-0.04839	-1.34915
H	-8.2047	-1.02471	-1.80293
H	-5.49197	4.323679	-0.16608
C	-10.959	-0.78918	-1.91233
C	-10.4955	0.140754	-1.01037
C	-12.9338	-0.39384	-0.74327

C	-12.3278	-1.08916	-1.76382
H	-10.33	-1.21576	-2.68763
H	-12.8676	-1.77876	-2.40777
S	-11.7799	0.640955	0.060593
C	-14.3027	-0.44384	-0.30449
C	-14.9801	0.420328	0.526964
C	-16.3216	0.048594	0.746334
C	-16.6941	-1.09901	0.088159
H	-14.5216	1.313088	0.942362
H	-17.0131	0.637475	1.342975
S	-15.3437	-1.74975	-0.80891
C	4.329211	0.172824	-0.46468
C	5.420208	0.999201	-0.25565
C	5.081765	2.375111	-0.01445
C	3.70705	2.841414	-0.00059
C	2.601196	1.947641	-0.22465
C	3.010926	0.642685	-0.44643
H	4.451174	-0.88963	-0.6522
Si	-2.05977	5.023637	0.096581
C	-2.15737	5.824763	1.78783
H	-2.17868	5.066842	2.577258
H	-1.29014	6.471382	1.962145
H	-3.05873	6.44101	1.880735
C	-2.04199	6.318188	-1.25801
H	-1.99212	5.847636	-2.24504
H	-2.94345	6.940125	-1.22109
H	-1.17434	6.979048	-1.15334
H	1.404207	4.496901	0.148709
S	5.131814	4.718605	0.429218
N	3.613435	4.148723	0.239773
N	5.968368	3.337307	0.214838
C	8.542031	-1.00322	-0.49998
C	9.254385	0.150423	-0.2012
C	6.77059	0.506064	-0.28121
C	7.163684	-0.79935	-0.54362
H	9.022163	-1.95749	-0.69655
H	6.458605	-1.59243	-0.77358
S	8.176772	1.504535	0.029629
C	13.14434	-0.08242	0.011458
C	12.77512	1.257468	0.160725
C	11.40062	1.467717	0.106055
C	10.66482	0.30411	-0.08169
H	13.52084	2.028326	0.312118

H	10.9365	2.44728	0.1863
S	11.71918	-1.07888	-0.1871
F	2.078518	-0.29556	-0.66757
C	-17.9912	-1.75776	0.086853
C	-18.8781	-1.54845	1.157084
C	-18.3788	-2.60822	-0.96465
C	-20.1053	-2.18015	1.104754
H	-18.585	-0.93057	2.002462
C	-19.6121	-3.25306	-0.97782
H	-17.6991	-2.75131	-1.80169
H	-19.8753	-3.90847	-1.80467
C	-20.4992	-3.02796	0.060028
C	16.68214	-0.73526	0.923198
C	16.3239	-1.99995	0.451589
C	17.26738	-3.0158	0.470945
C	18.53807	-2.74114	0.98644
C	18.87365	-1.47137	1.465588
C	17.93032	-0.44573	1.424731
C	14.45945	-0.61001	0.127779
H	17.05525	-4.02337	0.130319
H	18.17149	0.55682	1.768749
C	15.53903	0.19216	0.749586
O	15.53371	1.36471	1.083464
C	14.94205	-1.9106	-0.10958
C	14.33116	-2.93108	-0.85332
N	14.6282	-4.3082	-0.60752
O	14.62276	-5.1071	-1.53331
O	14.91349	-4.60271	0.557818
N	13.46676	-2.67012	-1.96977
O	12.62296	-3.50588	-2.26883
O	13.59677	-1.58802	-2.53923
H	-5.93439	-0.13457	-1.63096
C	-22.1701	-2.87602	1.6676
C	-21.8491	-3.5819	0.399091
C	-23.1377	-3.2924	-0.39751
H	-23.279	-3.9652	-1.24851
C	-23.6223	-2.79882	1.955815
C	-24.2231	-3.44111	0.680749
H	-25.1758	-2.98678	0.396633
N	-21.1589	-2.10168	2.049595
C	-21.1448	-1.19461	3.178249
H	-20.3292	-1.45884	3.859756
H	-20.9973	-0.16647	2.83076

H	-22.0914	-1.26711	3.716684
H	-23.9305	-3.31287	2.876961
H	-23.9309	-1.74761	2.069879
H	-24.4144	-4.50591	0.863402
H	-23.1035	-2.26362	-0.77988
H	-21.7946	-4.67525	0.565319
H	-7.45507	3.352475	0.373225
H	-9.73557	2.508669	0.109437
Cl	19.69845	-4.03449	1.017256
Cl	20.452256	-1.13186	2.108775

Table S4: Cartesian coordinates of **MSTD4**

Atom	X-axis	Y-axis	Z-axis
C	0.775387	2.249666	-0.07429
C	0.292474	3.549359	-0.04461
C	-1.11	3.646366	-0.10469
C	-1.70402	2.394107	-0.18068
C	-3.80783	3.581606	-0.25497
C	-3.1426	2.362814	-0.26121
C	-5.20293	3.403088	-0.35273
C	-5.60722	2.085449	-0.43146
S	-4.21588	1.013755	-0.37931
S	-0.56381	1.102152	-0.17697
C	-7.19382	0.217287	-0.907
C	-6.95407	1.553333	-0.5463
C	-8.07245	2.36528	-0.29499
C	-9.35784	1.872118	-0.41386
C	-9.59271	0.537502	-0.77429
C	-8.47853	-0.28012	-1.01057
H	-8.62641	-1.32837	-1.26107
H	-5.91356	4.225128	-0.39067
C	-11.3516	-1.09253	-1.63597
C	-10.9363	-0.00554	-0.90115
C	-13.3951	-0.47225	-0.70826
C	-12.7316	-1.3548	-1.52884
H	-10.6776	-1.66272	-2.2677
H	-13.2377	-2.15454	-2.06366
S	-12.2833	0.696805	-0.04107
C	-14.7915	-0.43764	-0.36559
C	-15.5248	0.581938	0.199994
C	-16.8787	0.248703	0.404903
C	-17.2053	-1.02394	0.001042

H	-15.0971	1.553153	0.43126
H	-17.609	0.948313	0.80259
S	-15.795	-1.84034	-0.6291
C	3.874561	0.015757	-0.08842
C	4.970999	0.860289	-0.04431
C	4.639107	2.258104	0.014936
C	3.265679	2.726818	0.014498
C	2.154621	1.813971	-0.04721
C	2.557036	0.48915	-0.08887
H	3.991698	-1.06279	-0.13114
Si	-2.489451	4.927466	-0.13353
C	-2.60762	5.9335	1.444171
H	-2.63926	5.28053	2.322074
H	-1.74183	6.597156	1.546286
H	-3.50931	6.556254	1.447899
C	-2.43868	6.043915	-1.63819
H	-2.39514	5.454074	-2.5592
H	-3.32668	6.684395	-1.68397
H	-1.55721	6.69411	-1.60999
H	0.971048	4.392882	0.014675
S	4.700804	4.640922	0.125562
N	3.177409	4.054671	0.075153
N	5.531014	3.240582	0.074138
C	8.093841	-1.15529	-0.15472
C	8.809031	0.032265	-0.08994
C	6.32188	0.367056	-0.06299
C	6.712668	-0.96312	-0.13986
H	8.573735	-2.12698	-0.22984
H	6.002532	-1.78283	-0.19396
S	7.73344	1.403571	-0.00206
C	12.70749	-0.12761	-0.14203
C	12.3216	1.214412	-0.15744
C	10.9419	1.398199	-0.13476
C	10.22207	0.21139	-0.0964
H	13.05732	2.00844	-0.17859
H	10.46081	2.372649	-0.16017
S	11.29579	-1.16014	-0.08401
F	1.616066	-0.46539	-0.14043
C	-18.4991	-1.68553	0.060811
C	-19.4629	-1.24112	0.982844
C	-18.8093	-2.77067	-0.77979
C	-20.682	-1.88899	0.997358
H	-19.2318	-0.43368	1.673281

C	-20.0374	-3.42302	-0.72278
H	-18.0713	-3.09987	-1.50763
H	-20.2384	-4.26355	-1.38268
C	-20.998	-2.97229	0.165551
C	16.33578	-0.62502	0.534611
C	15.94576	-1.94098	0.257751
C	16.87839	-2.96277	0.290985
C	18.19424	-2.65172	0.634686
C	18.59424	-1.34604	0.931751
C	17.64067	-0.31328	0.867619
C	14.03855	-0.6262	-0.06424
H	16.62578	-3.99735	0.088205
C	15.15221	0.263693	0.347447
O	15.12334	1.467139	0.518402
C	14.51445	-1.93731	-0.16093
C	13.84484	-3.06439	-0.67569
N	14.1464	-4.37531	-0.20111
O	14.02941	-5.34048	-0.94321
O	14.55753	-4.44689	0.963395
N	12.90989	-2.97615	-1.75774
O	12.05622	-3.84674	-1.87475
O	12.99577	-1.99286	-2.49331
H	-6.35338	-0.44366	-1.11171
C	-22.7808	-2.46415	1.563066
C	-22.3655	-3.45584	0.537507
C	-23.5988	-3.41305	-0.38795
H	-23.6718	-4.28231	-1.04796
C	-24.2496	-2.35997	1.730272
C	-24.7537	-3.31863	0.62271
H	-25.6907	-2.97814	0.17466
N	-21.8041	-1.60148	1.816346
C	-21.8757	-0.44862	2.690382
H	-21.1425	-0.54574	3.498092
H	-21.6592	0.462067	2.122422
H	-22.8747	-0.38214	3.124661
H	-24.6126	-2.63466	2.730351
H	-24.5777	-1.32329	1.55553
H	-24.9426	-4.30894	1.055548
H	-23.5516	-2.5132	-1.01537
H	-22.3161	-4.46965	0.9808
H	-7.92838	3.399867	0.006808
H	-10.2001	2.538977	-0.23474
Cl	19.343349	-3.95177	0.691744

Cl	20.230107	-0.99924	1.365414
Cl	18.110919	1.320236	1.190259

Table S5: Cartesian coordinates of **MSTD5**

Atom	X-axis	Y-axis	Z-axis
C	1.529281	2.282962	0.020948
C	1.053305	3.585591	0.022497
C	-0.34789	3.689043	-0.06031
C	-0.9471	2.43875	-0.12576
C	-3.04497	3.633033	-0.24804
C	-2.38426	2.412079	-0.22706
C	-4.43936	3.457444	-0.36449
C	-4.84639	2.140057	-0.43148
S	-3.45983	1.064827	-0.34267
S	0.185284	1.141143	-0.0831
C	-6.42824	0.273699	-0.92619
C	-6.19253	1.608707	-0.55918
C	-7.31317	2.419126	-0.3137
C	-8.59736	1.924957	-0.44316
C	-8.82819	0.591048	-0.80875
C	-7.71163	-0.22474	-1.04002
H	-7.85683	-1.27233	-1.2948
H	-5.14715	4.280589	-0.4257
C	-10.5792	-1.03746	-1.68888
C	-10.1701	0.045772	-0.94523
C	-12.6278	-0.43064	-0.76366
C	-11.9587	-1.30522	-1.58812
H	-9.90104	-1.60109	-2.3221
H	-12.4606	-2.10303	-2.12977
S	-11.5223	0.737725	-0.08498
C	-14.0253	-0.40464	-0.42389
C	-14.7658	0.609158	0.142325
C	-16.118	0.266883	0.344688
C	-16.4357	-1.00705	-0.06179
H	-14.3444	1.582608	0.376109
H	-16.8533	0.96096	0.742837
S	-15.0195	-1.81324	-0.69138
C	4.609962	0.02598	0.086995
C	5.71353	0.862211	0.115142
C	5.392954	2.263725	0.140129
C	4.02309	2.743341	0.119451

C	2.904926	1.838355	0.071963
C	3.296854	0.50958	0.067098
H	4.717829	-1.05419	0.071639
Si	-1.721985	4.974744	-0.12687
C	-1.85814	6.003003	1.435221
H	-1.898	5.362422	2.321882
H	-0.99453	6.669576	1.537015
H	-2.76084	6.62412	1.420669
C	-1.64633	6.071566	-1.64502
H	-1.59561	5.470362	-2.55827
H	-2.52982	6.716696	-1.70895
H	-0.76137	6.716885	-1.61422
H	1.735741	4.426271	0.078121
S	5.473346	4.647926	0.193393
N	3.945368	4.072854	0.146979
N	6.292661	3.239894	0.181716
C	8.809053	-1.19308	0.042291
C	9.541759	-0.01448	0.084434
C	7.058729	0.354638	0.109068
C	7.43166	-0.982	0.055785
H	9.274806	-2.17266	-0.01736
H	6.710771	-1.79298	0.01593
S	8.484662	1.373249	0.149387
C	13.43275	-0.27145	-0.01136
C	13.08268	1.081505	-0.02919
C	11.70928	1.302723	0.011686
C	10.95737	0.135636	0.066449
H	13.84117	1.853806	-0.06645
H	11.25533	2.290033	-0.01328
S	11.99455	-1.26435	0.07445
F	2.348794	-0.43885	0.033781
C	-17.7252	-1.67793	-0.0035
C	-18.6909	-1.24291	0.920824
C	-18.0283	-2.76258	-0.84707
C	-19.9056	-1.8992	0.935274
H	-18.4643	-0.43598	1.61333
C	-19.2519	-3.42364	-0.79037
H	-17.2888	-3.08435	-1.57669
H	-19.4479	-4.26361	-1.45253
C	-20.2145	-2.98249	0.10044
C	17.05031	-0.86317	0.584928
C	16.62353	-2.17858	0.35907
C	17.52953	-3.22789	0.404457

C	18.8528	-2.92512	0.701919
C	19.28715	-1.62616	0.935246
C	18.36934	-0.57925	0.867486
C	14.74935	-0.80583	0.044755
H	17.25885	-4.26717	0.255611
C	15.90277	0.059119	0.40609
O	15.92651	1.267376	0.548071
C	15.18416	-2.13487	-0.03335
C	14.47224	-3.24828	-0.5184
N	14.75352	-4.56246	-0.03856
O	14.61341	-5.52917	-0.77481
O	15.17184	-4.63608	1.122954
N	13.52738	-3.15289	-1.59181
O	12.65113	-4.00384	-1.68434
O	13.62886	-2.18482	-2.34505
H	-5.58542	-0.38505	-1.12818
C	-21.9997	-2.49231	1.501781
C	-21.5784	-3.47716	0.471703
C	-22.8113	-3.43751	-0.45453
H	-22.8798	-4.30488	-1.11764
C	-23.4693	-2.3941	1.666107
C	-23.9676	-3.35186	0.555205
H	-24.9059	-3.01481	0.107284
N	-21.0278	-1.6226	1.756371
C	-21.1066	-0.47387	2.634695
H	-20.3705	-0.56735	3.440237
H	-20.9001	0.441338	2.070181
H	-22.105	-0.41788	3.072138
H	-23.8344	-2.67293	2.664384
H	-23.8015	-1.35828	1.493104
H	-24.1518	-4.34445	0.984913
H	-22.7678	-2.53523	-1.07879
H	-21.5218	-4.49332	0.908843
H	-7.17169	3.452556	-0.0065
H	-9.44175	2.590119	-0.26763
F	19.75411	-3.89956	0.77271
F	20.56267	-1.38461	1.215337
F	18.79962	0.656742	1.064797

Table S6: Cartesian coordinates of **MSTD6**

Atom	**X-axis**	**Y-axis**	**Z-axis**

C	0.828015	2.251728	-0.04458
C	0.33778	3.548239	-0.00791
C	-1.06513	3.637569	-0.0679
C	-1.65202	2.382525	-0.15099
C	-3.76129	3.560322	-0.22116
C	-3.09086	2.344553	-0.23286
C	-5.15545	3.376493	-0.32115
C	-5.55406	2.057671	-0.40666
S	-4.15841	0.991541	-0.35864
S	-0.50438	1.097059	-0.15387
C	-7.13607	0.186895	-0.8906
C	-6.89937	1.522151	-0.52519
C	-8.01946	2.33143	-0.27306
C	-9.30375	1.836744	-0.39612
C	-9.53565	0.503023	-0.76155
C	-8.41993	-0.31221	-0.99834
H	-8.5657	-1.35981	-1.25283
H	-5.86941	4.19578	-0.35567
C	-11.2924	-1.12482	-1.63325
C	-10.8787	-0.0405	-0.89342
C	-13.3379	-0.50611	-0.70913
C	-12.6729	-1.38648	-1.5309
H	-10.6169	-1.69304	-2.26515
H	-13.178	-2.1838	-2.07026
S	-12.2272	0.65949	-0.03436
C	-14.7352	-0.47016	-0.37083
C	-15.4687	0.551465	0.191352
C	-16.8232	0.22029	0.393409
C	-17.1505	-1.05247	-0.00998
H	-15.0402	1.52263	0.42131
H	-17.5534	0.921785	0.787973
S	-15.7394	-1.87208	-0.63472
C	3.944751	0.040881	-0.07144
C	5.033818	0.893578	-0.02505
C	4.691316	2.288296	0.040427
C	3.314704	2.746417	0.044024
C	2.210577	1.825324	-0.02026
C	2.622716	0.504254	-0.06801
H	4.070441	-1.03652	-0.12
Si	-2.450268	4.912352	-0.09089
C	-2.57494	5.908014	1.492786
H	-2.60585	5.249431	2.366511
H	-1.71171	6.574073	1.600715

H	-3.47875	6.527646	1.498812
C	-2.40335	6.037301	-1.58916
H	-2.35572	5.452919	-2.51344
H	-3.29445	6.673625	-1.63244
H	-1.52524	6.691776	-1.55623
H	1.011326	4.395443	0.055939
S	4.734966	4.670936	0.161571
N	3.216363	4.073363	0.110692
N	5.575603	3.277645	0.102627
C	8.181696	-1.08665	-0.14354
C	8.880608	0.109551	-0.08575
C	6.390452	0.412851	-0.04732
C	6.796828	-0.91195	-0.12231
H	8.673331	-2.05257	-0.2176
H	6.097199	-1.7411	-0.16958
S	7.788647	1.466697	0.004507
C	12.78246	0.028775	-0.14553
C	12.36932	1.360242	-0.17195
C	10.98502	1.515075	-0.14925
C	10.29203	0.314121	-0.09896
H	13.08628	2.171056	-0.19976
H	10.48356	2.478849	-0.18299
S	11.3944	-1.03387	-0.07673
F	1.689224	-0.45712	-0.12299
C	-18.4461	-1.70978	0.046572
C	-19.4136	-1.26155	0.963786
C	-18.7567	-2.79453	-0.79427
C	-20.6341	-1.90597	0.970812
H	-19.1836	-0.45459	1.65504
C	-19.9866	-3.44338	-0.7443
H	-18.0161	-3.12651	-1.51823
H	-20.1867	-4.28336	-1.40498
C	-20.9504	-2.98761	0.13837
C	16.41304	-0.36592	0.546608
C	16.08042	-1.68849	0.252506
C	17.07714	-2.6587	0.286858
C	18.35849	-2.26628	0.655171
C	18.67101	-0.93966	0.953129
C	17.68316	0.036653	0.891544
C	14.12826	-0.43245	-0.0597
H	16.89189	-3.70776	0.085469
H	17.91824	1.079523	1.084444
C	15.21012	0.485765	0.358669

O	15.17984	1.689544	0.540608
C	14.64835	-1.73017	-0.16457
C	14.01648	-2.87715	-0.68234
N	14.36451	-4.179	-0.21738
O	14.22317	-5.15085	-0.94462
O	14.83577	-4.23514	0.926579
N	13.06352	-2.80708	-1.75169
O	12.22465	-3.69201	-1.85958
O	13.12305	-1.82001	-2.4848
H	-6.29416	-0.47197	-1.0959
C	-22.7373	-2.47206	1.528149
C	-22.3198	-3.46616	0.50732
C	-23.5543	-3.43004	-0.41646
H	-23.6235	-4.30094	-1.07433
C	-24.2057	-2.3776	1.701924
C	-24.7083	-3.33927	0.596198
H	-25.6467	-3.00204	0.149102
N	-21.7625	-1.61399	1.784726
C	-21.8339	-0.45878	2.657097
H	-21.105	-0.55933	3.467853
H	-21.609	0.448574	2.087419
H	-22.8349	-0.38661	3.085814
H	-24.5597	-2.65356	2.704585
H	-24.5397	-1.34287	1.528869
H	-24.8935	-4.32968	1.030009
H	-23.5122	-2.53163	-1.04618
H	-22.271	-4.47512	0.960604
H	-7.87761	3.365195	0.032432
H	-10.1474	2.501864	-0.21671
N	19.34008	-3.35054	0.834284
O	19.91852	-3.39256	1.903373
O	19.44395	-4.15017	-0.07603
N	20.04452	-0.50235	1.207906
O	20.94109	-1.12085	0.6605
O	20.188	0.483701	1.911569

Table S7: Cartesian coordinates of **MSTD7**

Atom	X-axis	Y-axis	Z-axis
C	0.243332	2.270535	-0.09533
C	-0.24196	3.569722	-0.09751
C	-1.64405	3.662593	-0.16741

C	-2.23505	2.407483	-0.21877
C	-4.34073	3.588875	-0.32424
C	-3.67313	2.371412	-0.30374
C	-5.73499	3.405493	-0.42187
C	-6.13613	2.085418	-0.47508
S	-4.74302	1.017894	-0.39789
S	-1.09275	1.118256	-0.17961
C	-7.71864	0.208595	-0.92915
C	-7.48158	1.548744	-0.58175
C	-8.6013	2.360539	-0.33527
C	-9.88562	1.863017	-0.4457
C	-10.1178	0.524315	-0.79267
C	-9.0023	-0.29287	-1.0248
H	-9.14822	-1.34377	-1.26517
H	-6.44743	4.224867	-0.47881
C	-11.8752	-1.11919	-1.63171
C	-11.46	-0.02368	-0.9088
C	-13.9158	-0.49684	-0.69929
C	-13.2532	-1.38486	-1.51532
H	-11.2022	-1.69298	-2.26123
H	-13.7588	-2.19141	-2.04041
S	-12.8047	0.682613	-0.049
C	-15.3099	-0.46381	-0.35018
C	-16.0403	0.554279	0.223575
C	-17.3922	0.220667	0.434674
C	-17.7217	-1.05081	0.027591
H	-15.6108	1.524237	0.45663
H	-18.1193	0.919832	0.838993
S	-16.3149	-1.86509	-0.61415
C	3.347546	0.044293	-0.03983
C	4.441129	0.892012	-0.01611
C	4.106337	2.289909	0.00646
C	2.732423	2.755451	-0.01066
C	1.623364	1.838735	-0.05151
C	2.028276	0.514447	-0.05591
H	3.467302	-1.03474	-0.05409
Si	-3.025492	4.940593	-0.22861
C	-3.15023	5.980587	1.326168
H	-3.17995	5.347361	2.218481
H	-2.28772	6.650483	1.414421
H	-4.05472	6.599136	1.314862
C	-2.97443	6.023141	-1.75754
H	-2.92905	5.413942	-2.66576

H	-3.86347	6.660962	-1.81772
H	-2.0943	6.675551	-1.74247
H	0.434685	4.415722	-0.05308
S	4.162922	4.674734	0.054249
N	2.641232	4.084225	0.014047
N	4.995933	3.2758	0.042868
C	7.571607	-1.11563	-0.08754
C	8.280781	0.07499	-0.05485
C	5.79432	0.40117	-0.02354
C	6.188453	-0.92844	-0.07013
H	8.05457	-2.08708	-0.14382
H	5.481512	-1.75201	-0.10217
S	7.201857	1.443486	0.007056
C	12.17815	-0.06703	-0.14883
C	11.79001	1.268994	-0.19805
C	10.40705	1.448581	-0.16332
C	9.695631	0.261708	-0.07946
H	12.51921	2.067152	-0.2567
H	9.921907	2.419806	-0.21538
S	10.77468	-1.1035	-0.03616
F	1.089919	-0.44326	-0.08441
C	-19.0148	-1.71055	0.090716
C	-19.9806	-1.26124	1.009378
C	-19.3262	-2.80124	-0.74346
C	-21.1978	-1.91021	1.023878
H	-19.7512	-0.4502	1.696034
C	-20.5534	-3.45373	-0.6855
H	-18.5874	-3.1352	-1.46832
H	-20.7528	-4.29775	-1.34114
C	-21.5156	-2.99691	0.19883
C	15.81157	-0.56253	0.506646
C	15.444	-1.8624	0.15471
C	16.40942	-2.85804	0.083799
C	17.72099	-2.52541	0.40307
C	18.09507	-1.23561	0.761578
C	17.11698	-0.24774	0.815871
C	13.51595	-0.56318	-0.08054
H	16.18838	-3.88568	-0.17989
C	14.62187	0.330439	0.316969
O	14.6279	1.538119	0.444066
C	13.99934	-1.86659	-0.21187
C	13.33119	-3.00224	-0.71516
N	13.65082	-4.30343	-0.23428

O	13.44425	-5.28874	-0.9272
O	14.1714	-4.34775	0.890071
N	12.3613	-2.90885	-1.7659
O	11.50127	-3.77415	-1.86282
O	12.43121	-1.92035	-2.49669
H	-6.87701	-0.45192	-1.13017
C	-23.2966	-2.47497	1.591526
C	-22.8819	-3.47627	0.576968
C	-24.1239	-3.45247	-0.33747
H	-24.193	-4.32813	-0.98873
C	-24.7635	-2.39425	1.78271
C	-25.2704	-3.36217	0.684086
H	-26.2133	-3.02983	0.242985
N	-22.3256	-1.61569	1.841088
C	-22.3971	-0.45566	2.708543
H	-21.6661	-0.55261	3.517547
H	-22.1742	0.448342	2.133237
H	-23.3973	-0.38269	3.138975
H	-25.0998	-2.67211	2.790708
H	-25.1082	-1.36279	1.613499
H	-25.449	-4.35146	1.12297
H	-24.0918	-2.55831	-0.97372
H	-22.8306	-4.47973	1.0422
H	-8.45878	3.398126	-0.04331
H	-10.7291	2.529397	-0.27037
N	18.70349	-3.62181	0.444819
O	19.56954	-3.55303	1.298423
O	18.55146	-4.5272	-0.3527
N	19.49477	-0.86841	1.026034
O	20.29183	-1.09687	0.140187
O	19.71662	-0.33507	2.09523
N	17.50121	1.133903	1.159607
O	16.98131	1.612198	2.142764
O	18.31923	1.660889	0.427899

Table S8: Calculated energies (E) and energy gap (ΔE) for **(DTS(FBTTh$_2$)$_2$R1** and **MSTD2-MSTD7**)

Compounds	**E** $_{LUMO+1}$	**E** $_{HOMO-1}$	**ΔE (*eV*)**	**E** $_{LUMO+2}$	**E** $_{HOMO+2}$	**ΔE (*eV*)**
DTS(FBTTh$_2$)$_2$R1	-2.551	-5.611	3.06	-1.534	-6.041	4.507
MSTD2	-2.651	-5.461	2.81	-2.216	-5.289	3.073
MSTD3	-2.704	-5.360	2.656	-2.385	-5.858	3.385
MSTD4	-2.740	-5.382	2.642	-2.452	-5.874	3.422
MSTD5	-2.706	-5.358	2.652	-2.360	-5.863	3.503
MSTD6	-2.776	-5.445	2.669	-2.671	-5.907	3.236

MSTD7	-2.751	-5.506	2.755	-2.743	-5.929	3.186

E= energy, ΔE(e*V*)= E_{LUMO}-E_{HOMO}; HOMO= highest occupied molecular orbital; LUMO= lowest unoccupied molecular orbital, MO, molecular orbital, Units in e*V*

Table S9: Calculated global reactivity parameters using energies of HOMO and LUMO orbitals of studied compound (**DTS(FBTTh$_2$)$_2$R1** and **MSTD2- MSTD7**)

Compounds	*IP*	*EA*	*X*	*η*	*μ*	*ω*	σ
DTS(FBTTh$_2$)$_2$R1	0.188104	0.102469	0.14528617	0.042818	-0.14529	0.246489	11.67746
MSTD2	0.175346	0.105582	0.1404637	0.034882	-0.14046	0.28281	14.33398
MSTD3	0.179225	0.104203	0.14171432	0.0037511	-0.14171	0.267695	13.32948
MSTD4	0.181187	0.10335	0.142268	0.038918	-0.14227	0.260034	12.84739
MSTD5	0.179397	0.103804	0.14160038	0.037796	-0.1416	0.265246	13.22881
MSTD6	0.184506	0.114325	0.14941547	0.03509	-0.14942	0.318108	14.24898
MSTD7	0.186569	0.12179	0.15417947	0.032389	-0.15418	0.36696	15.4371

IP= ionization potential, *EA*= electron affinity, *X*= electro negativity, *μ* =chemical potential, *η* =global hardness, σ = global softness and *ω*= global electrophilicity. Units in Hartree (E_h)

Table S10: Natural bond orbital (NBO) analysis of investigated compound **DTS(FBTTh$_2$)$_2$R1**by using M06 6-31G(d,p).

Donor(i)	Type	Acceptor(j)	Type	E(2)[a] [kcal/mol]	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C11-C12	π	C13-N20	π*	26.73	0.27	0.080
C39-C40	π	C38-N54	π*	26.73	0.27	0.080
C15-C16	π	C14-N19	π*	25.38	0.26	0.076
C35-C36	π	C39-C40	π*	21.30	0.30	0.073
C3-C4	π	C1-C2	π*	19.76	0.30	0.071
C1-C2	π	C39-C40	π*	18.01	0.30	0.068
C11-C12	π	C15-C16	π*	17.53	0.32	0.067
C21-C22	π	C23-C24	π*	16.59	0.31	0.066
C28-C29	π	C30-C31	π*	15.76	0.32	0.065
C11-C12	π	C7-C8	π*	14.83	0.32	0.062
C15-C16	π	C21-C22	π*	12.71	0.30	0.057
C14-N19	π	C15-C16	π*	9.90	0.38	0.057
C13-N20	π	C11-C12	π*	8.61	0.37	0.053
C39-C40	π	C39-C40	π*	1.02	0.31	0.016
C5-C6	π	C5-C6	π*	0.68	0.30	0.013
N20-S51	σ	C12-C13	σ*	8.32	1.27	0.092
C3-Si42	σ	C4-S10	σ*	7.98	0.72	0.068
C70-H71	σ	C63-S69	σ*	6.47	0.72	0.061
C28-C29	σ	C23-C28	σ*	5.39	1.26	0.074
C23-C24	σ	C23-C28	σ*	5.17	1.26	0.072
C21-C24	σ	C23-C28	σ*	4.96	1.22	0.070
C5-C7	σ	C8-C12	σ*	4.16	1.21	0.063
C1-C39	σ	C1-C2	σ*	3.99	1.29	0.064
C5-C6	σ	C5-C7	σ*	3.45	1.29	0.060
C36-C37	σ	C37-N55	σ*	3.04	1.20	0.054

C58-C59	σ	C56-H60	σ*	2.93	1.18	0.053
Si42-C43	σ	Si42-C47	σ*	2.45	0.77	0.039
C12-C13	σ	C13-C14	σ*	2.14	1.19	0.045
C29-H32	σ	C28-C29	σ*	1.96	1.13	0.042
C64-C65	σ	C64-H67	σ*	1.09	1.13	0.031
C38-N54	σ	C39-C40	σ*	0.98	1.47	0.034
C4-C6	σ	C6-S9	σ*	0.71	0.95	0.023
C7-C8	σ	C6-S9	σ*	0.50	0.95	0.020
S9	LP(2)	C5-C6	π*	27.05	0.28	0.078
S27	LP(2)	C23-C24	π*	24.61	0.28	0.074
S62	LP(2)	C56-C57	π*	24.61	0.28	0.074
S51	LP(2)	C14-N19	π*	23.33	0.26	0.071
S51	LP(2)	C13-N20	π*	22.71	0.26	0.070
S9	LP(2)	C7-C8	π*	20.82	0.28	0.068
F79	LP(3)	C39-C40	π*	20.52	0.46	0.094
N19	LP(1)	C13-C14	σ*	7.67	0.94	0.076
F78	LP(2)	C11-C16	σ*	6.85	1.01	0.074
F78	LP(2)	C11-C12	σ*	5.48	1.04	0.067
N20	LP(1)	N19-S51	σ*	4.72	0.67	0.050
S51	LP(1)	C13-N20	σ*	3.25	1.18	0.055
S9	LP(1)	C5-C6	σ*	2.79	1.23	0.052
S27	LP(1)	C23-C24	σ*	2.44	1.25	0.049
S27	LP(1)	C21-C22	σ*	1.92	1.25	0.044
F79	LP(1)	C4-S10	σ*	0.81	1.28	0.029
N54	LP(1)	C38-C39	σ*	0.57	0.97	0.021

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S11: Natural bond orbital (NBO) analysis of investigated compound **MSTD2** by using M06 6-31g(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2) [a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C1-C2	π	C83-C113	π*	26.69	0.31	0.082
C7-C8	π	C70-C73	π*	23.18	0.29	0.076
C26-C27	π	C78-C79	π*	20.81	0.3	0.07
C36-N51	π	C107-C108	π*	19.14	0.29	0.068
C53-C54	π	C103-C104	π*	18.15	0.3	0.067
C68-C69	π	C62-C63	π*	16.88	0.29	0.064
C71-C76	π	C19-C20	π*	14.97	0.28	0.059
C80-C81	π	C14-C15	π*	12.58	0.32	0.059
C83-C113	π	C68-C69	π*	10.79	0.32	0.055
C88-O89	π	C37-C38	π*	8.83	0.37	0.054
C90-C91	π	C83-C113	π*	6.76	0.35	0.044
N92-O93	π	N115-O117	π*	3.28	0.18	0.024

C107-C108	π	C71-C76	π*	0.72	0.28	0.013
N115-O117	π	C90-C91	π*	0.53	0.33	0.012
C1-C2	σ	C36-C37	σ*	8.35	1.27	0.092
C1-C2	σ	C4-S10	σ*	7.97	0.72	0.068
C1-S10	σ	C71-N96	σ*	6.01	1.16	0.075
C2-C3	σ	C20-S25	σ*	5.27	0.74	0.056
C3-Si40	σ	C60-C113	σ*	4.99	1.3	0.072
C5-C7	σ	C28-C29	σ*	4.46	1.29	0.068
C7-H18	σ	C14-C15	σ*	4.19	1.1	0.061
C11-H95	σ	C79-C80	σ*	3.95	1.11	0.059
C20-S25	σ	C21-C26	σ*	3.41	1.19	0.057
C28-H31	σ	C56-H58	σ*	2.99	1.18	0.053
C41-H44	σ	C62-C63	σ*	2.35	1.3	0.049
C60-S66	σ	C71-N96	σ*	2.08	1.17	0.044
C61-C62	σ	C11-C12	σ*	1.99	1.31	0.046
C77-C78	σ	C79-C80	σ*	1.33	1.26	0.037
C81-H86	σ	C70-C73	σ*	1.09	1.13	0.031
C83-C90	σ	C14-C15	σ*	0.99	1.1	0.029
C113-H114	σ	Si40-C45	σ*	0.52	0.77	0.018
N115-O117	σ	C29-S32	σ*	0.51	0.95	0.02
S9	LP(1)	N115-O116	π*	21.34	0.74	0.113
S50	LP(1)	C91-N92	π*	13.92	0.61	0.082
O94	LP(2)	C7-C8	π*	2.08	1.26	0.046
O117	LP(2)	C113-H114	π*	0.54	1.09	0.022
S9	LP(2)	N115-O117	σ*	177.19	0.16	0.152
S50	LP(2)	C53-C54	σ*	23.72	0.28	0.072
N96	LP(1)	N115-O117	σ*	1.97	0.18	0.019
O117	LP(2)	C90-C91	σ*	0.51	0.33	0.012

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S12: Natural bond orbital (NBO) analysis of investigated compound **MSTD3** by using M06 6-31G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2) [a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C 60 - C 61	π	C 83 - C 113	π*	27.99	0.3	0.083
C 33 - C 34	π	C 35 - N 52	π*	26.19	0.26	0.077
C 62 - C 63	π	C 60 - C 61	π*	24.75	0.3	0.078
C 83 - C 113	π	C 88 - C 89	π*	23.94	0.29	0.075
C 103 - C 104	π	C 107 - C 108	π*	22.82	0.29	0.074
C 78 - C 79	π	C 77 - C 82	π*	21.25	0.31	0.073
C 3 - C 4	π	C 1 - C 2	π*	20.75	0.3	0.073
C 105 - C 106	π	C 107 - C 108	π*	19.13	0.29	0.068
C 107 - C 108	π	C 103 - C 104	π*	18.17	0.3	0.067

C 26 - C 27	π	C 28 - C 29	π*	16.9	0.31	0.067
C 37 - C 38	π	C 1 - C 2	π*	14.46	0.32	0.062
C 68 - C 69	π	C 28 - C 29	π*	12.44	0.29	0.053
C 36 - N 51	π	C 37 - C 38	π*	8.85	0.37	0.054
N 115 - O 117	π	C 88 - C 89	π*	0.66	0.51	0.018
S 50 - N 51	σ	C 36 - C 37	σ*	8.35	1.27	0.092
C 3 -Si 40	σ	C 4 - S 10	σ*	7.95	0.72	0.068
C 107 - C 108	σ	N 94 - C 106	σ*	6.38	1.16	0.077
C 22 - H 24	σ	C 21 - S 25	σ*	5.28	0.74	0.056
C 19 - C 20	σ	C 15 - C 20	σ*	4.87	1.25	0.07
C 105 - C 106	σ	C 104 - C 105	σ*	3.61	1.28	0.061
C 77 - C 86	σ	C 77 - C 82	σ*	2.99	1.27	0.055
C 5 - C 6	σ	C 5 -Si 40	σ*	2.1	0.99	0.041
C 3 - C 4	σ	C 3 -Si 40	σ*	2.08	0.99	0.041
C 19 - C 20	σ	C 14 - C 15	σ*	2.04	1.31	0.046
C 45 - H 46	σ	Si 40 - C 41	σ*	2.01	0.77	0.035
C 77 - C 78	σ	C 78 - C 88	σ*	1.98	1.16	0.043
C 89 - N 115	σ	C 88 - C 89	σ*	1.67	1.43	0.044
C 60 - C 61	σ	C 61 - H 64	σ*	1.41	1.19	0.037
C 27 - C 28	σ	C 27 - H 30	σ*	1.21	1.13	0.033
C 70 - H 74	σ	C 70 - C 73	σ*	1.11	1.13	0.032
C 45 - H 48	σ	Si 40 - C 45	σ*	0.52	0.77	0.018
C 26 - C 27	σ	C 29 - S 32	σ*	0.51	0.95	0.02
O 116	LP (3)	N 115 - O 117	π*	177.93	0.16	0.153
S 25	LP (2)	C 19 - C 20	π*	22.93	0.29	0.072
O 91	LP (2)	N 115 - O 117	π*	2.05	0.18	0.019
O 117	LP (2)	C 88 - C 89	π*	0.55	0.33	0.013
O 87	LP (2)	C 77 - C 86	σ*	21.89	0.75	0.116
O 92	LP (1)	C 89 - N 90	σ*	4.37	1.13	0.064
S 59	LP (1)	C 55 - C 56	σ*	2.01	1.25	0.045
Cl 102	LP (2)	C 77 - C 82	σ*	0.51	0.93	0.02

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S13: Natural bond orbital (NBO) analysis of investigated compound **MSTD4** by using M06 6-31G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2) [a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C60-C61	π	C83-C116	π*	27.48	0.3	0.082
C62-C63	π	C60-C61	π*	24.48	0.3	0.078
C108-C109	π	C106-C107	π*	22.85	0.29	0.075
C3-C4	π	C1-C2	π*	20.71	0.3	0.072
C106-C107	π	C108-C109	π*	18.49	0.29	0.069
C19-C20	π	C21-C22	π*	17.08	0.31	0.067

C7-C8	π	C5-C6	π*	16.54	0.3	0.066
C26-C27	π	C21-C22	π*	15.03	0.31	0.063
C37-C38	π	C1-C2	π*	14.42	0.32	0.061
C19-C20	π	C14-C15	π*	12.27	0.32	0.059
C28-C29	π	C68-C69	π*	10.81	0.32	0.055
N89-O90	π	C87-C88	π*	3.74	0.49	0.041
C87-C88	π	N92-O93	π*	3.25	0.18	0.024
C87-C88	π	C87-C88	π*	0.52	0.33	0.012
S50-N51	σ	C36-C37	σ*	8.34	1.27	0.092
C116-H117	σ	C83-C85	σ*	6.75	1.01	0.074
C61-H64	σ	C60-S66	σ*	5.21	0.73	0.055
C36-C37	σ	C38-F67	σ*	4.99	0.99	0.063
C11-H95	σ	C12-C13	σ*	4.19	1.1	0.061
C97-H100	σ	C71-N96	σ*	4.11	0.99	0.057
C83-C87	σ	C78-C79	σ*	3.99	1.26	0.064
C2-C3	σ	C3-C4	σ*	3.69	1.25	0.061
C63-S66	σ	C62-H65	σ*	3.44	1.13	0.056
C68-C69	σ	C29-S32	σ*	3.12	0.91	0.048
C27-C28	σ	C26-C27	σ*	2.82	1.28	0.054
C61-C62	σ	C62-C63	σ*	2.68	1.27	0.052
C1-C37	σ	C35-C36	σ*	1.98	1.2	0.044
C36-N51	σ	C35-C36	σ*	1.69	1.38	0.043
C29-C68	σ	C27-C28	σ*	1.42	1.26	0.038
C70-H74	σ	C70-C73	σ*	1.11	1.13	0.032
C83-C85	σ	C77-C85	σ*	0.61	1.15	0.024
C1-C2	σ	C4-S10	σ*	0.5	0.95	0.02
O94	LP(3)	N92-O93	π*	177.6	0.16	0.153
S10	LP(2)	C1-C2	π*	20.45	0.28	0.068
O90	LP(2)	N92-O93	π*	2.01	0.18	0.019
O93	LP(2)	C87-C88	π*	0.52	0.33	0.012
O86	LP(2)	C77-C85	σ*	21.76	0.75	0.116
F67	LP(2)	C33-C38	σ*	6.92	1.01	0.075
N96	LP(1)	C97-H98	σ*	2.03	0.68	0.037
F67	LP(1)	C33-C38	σ*	0.5	1.6	0.025

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S14: Natural bond orbital (NBO) analysis of investigated compound **MSTD5** by using M06 6-31G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kJ/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C60-C61	π	C83-C116	π*	27.18	0.3	0.082
C33-C34	π	C35-N52	π*	26.11	0.26	0.077
C14-C15	π	C11-C16	π*	20.26	0.3	0.071

C5-C6	π	C7-C8	π*	17.93	0.31	0.068
N89-O90	π	N89-O90	π*	7.43	0.35	0.055
C87-C88	π	C83-C116	π*	6.69	0.35	0.044
C83-C116	π	C87-C88	π*	6.69	0.35	0.044
C87-C88	π	C87-C88	π*	0.58	0.33	0.013
S50-N51	σ	C36-C37	σ*	8.34	1.27	0.092
S50-N52	σ	C34-C35	σ*	8.3	1.28	0.092
C5-Si40	σ	C6-S9	σ*	8.29	0.71	0.069
C3-Si40	σ	C4-S10	σ*	7.95	0.72	0.068
C61-H64	σ	C60-S66	σ*	5.21	0.73	0.055
C14-C15	σ	C13-H101	σ*	2.23	1.15	0.045
C34-C35	σ	C35-C36	σ*	2.21	1.2	0.046
N96-C107	σ	C97-H99	σ*	0.52	1.21	0.023
C1-S10	σ	C1-C2	σ*	0.51	1.23	0.022
C6-S9	σ	C7-C8	σ*	0.51	1.27	0.023
C21-C22	σ	C20-S25	σ*	0.51	0.94	0.02
C26-C27	σ	C29-S32	σ*	0.51	0.94	0.02
C41-H44	σ	Si40-C41	σ*	0.51	0.77	0.018
C45-H47	σ	Si40-C45	σ*	0.51	0.77	0.018
C1-C2	σ	C4-S10	σ*	0.5	0.95	0.02
O94	LP(3)	N92-O93	π*	177.56	0.16	0.152
O91	LP(3)	N89-O90	π*	163.78	0.16	0.149
N96	LP(1)	C71-C76	π*	39.23	0.3	0.1
S32	LP(2)	C28-C29	π*	23.18	0.29	0.073
O90	LP(2)	C88-N89	σ*	14.35	0.61	0.084
O94	LP(2)	C88-N92	σ*	14.32	0.57	0.081
O91	LP(2)	C88-N89	σ*	13.8	0.61	0.082
O90	LP(2)	C87-C88	σ*	0.59	0.91	0.021
N51	LP(1)	C36-C37	σ*	0.58	0.97	0.021
O93	LP(2)	C87-C88	π*	0.51	0.33	0.012

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S15: Natural bond orbital (NBO) analysis of investigated compound **MSTD6** by using M06 6-31G(d,p).

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kJ/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[e](a.u)**
C60-C61	π	C83-C117	π*	30.34	0.3	0.085
C33-C34	π	C35-N52	π*	26.4	0.26	0.078
C62-C63	π	C60-C61	π*	26.16	0.29	0.08
C77-C82	π	C86-O87	π*	17.06	0.3	0.068
C60-C61	π	C62-C63	π*	17.05	0.29	0.063

C33-C34	π	C55-C56	π*	14.48	0.29	0.06
C37-C38	π	C1-C2	π*	14.47	0.32	0.061
C80-C81	π	N104-O106	π*	14.46	0.18	0.048
C35-N52	π	C36-N51	π*	14.14	0.34	0.066
C3-C4	π	C5-C6	π*	13.84	0.3	0.059
C12-C13	π	C7-C8	π*	13.53	0.28	0.056
C88-C89	π	N119-O121	π*	2.91	0.18	0.023
C109-C110	π	C109-C110	π*	0.71	0.28	0.013
N119-O121	π	C88-C89	π*	0.67	0.51	0.018
C37-C38	π	C37-C38	π*	0.62	0.31	0.013
C60-C61	π	C83-C117	π*	30.34	0.3	0.085
S50-N51	σ	C36-C37	σ*	8.36	1.27	0.092
C83-C86	σ	C77-C82	σ*	3.46	1.27	0.059
C5-C6	σ	C5-C7	σ*	3.45	1.28	0.06
C11-C16	σ	C11-C12	σ*	3.44	1.29	0.06
C13-C14	σ	C14-C15	σ*	3.44	1.29	0.06
C53-C54	σ	C56-H58	σ*	3.02	1.18	0.053
C73-C76	σ	C70-C73	σ*	3.02	1.31	0.056
C79-C80	σ	C78-C79	σ*	3.02	1.32	0.057
C41-H42	σ	Si40-C45	σ*	2.02	0.77	0.035
C83-C86	σ	C117-H118	σ*	2.02	1.09	0.042
C68-C69	σ	C70-H74	σ*	1.99	1.15	0.043
C21-C22	σ	C22-H24	σ*	1.53	1.18	0.038
C26-C27	σ	C27-H30	σ*	1.53	1.18	0.038
C6-S9	σ	C7-C8	σ*	0.51	1.27	0.023
C21-C22	σ	C20-S25	σ*	0.51	0.94	0.02
O93	LP(2)	C87-C88	π*	0.51	0.33	0.012
O105	LP(3)	N104-O106	π*	186.34	0.17	0.16
O102	LP(3)	N101-O103	π*	162.34	0.18	0.154
N94	LP(1)	C71-C76	π*	39.28	0.3	0.1
N94	LP(1)	C109-C110	π*	38.64	0.3	0.099
O102	LP(2)	C81-N101	σ*	15.08	0.58	0.083
F67	LP(2)	C37-C38	σ*	5.57	1.03	0.068
O91	LP(2)	N119-O121	π*	2.01	0.18	0.019
O102	LP(3)	N101-O103	σ*	0.53	0.71	0.02
O106	LP(2)	C80-C81	σ*	0.53	0.85	0.019
F67	LP(1)	C33-C38	σ*	0.5	1.61	0.025
O120	LP(3)	N119-O120	σ*	0.5	0.72	0.02

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S16: Natural bond orbital (NBO) analysis of investigated compound **MSTD67** by using M06 6-31G(d,p).

Donor(i)	Type	Accepto(j)	Type	E(2)[a] [kJ/mol]	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C60-C61	π	C83-C118	π*	32.77	0.3	0.09
C80-C81	π	N103-O104	π*	29.68	0.16	0.065
C33-C34	π	C55-C56	π*	14.24	0.3	0.059
C35-N52	π	C36-N51	π*	14.17	0.34	0.066
C87-C88	π	C83-C118	π*	6.72	0.35	0.045
C85-O86	π	C77-C82	π*	4.05	0.43	0.04
C85-O86	π	C83-C118	π*	3.45	0.43	0.037
C87-C88	π	N89-O91	π*	1.37	0.18	0.016
C62-C63	π	C62-C63	π*	1.11	0.29	0.016
C35-N52	π	C35-N52	π*	0.92	0.34	0.017
C3-C4	π	C3-C4	π*	0.89	0.29	0.015
C71-C76	π	C71-C76	π*	0.73	0.28	0.013
C110-C111	π	C110-C111	π*	0.71	0.28	0.013
C37-C38	π	C37-C38	π*	0.67	0.31	0.013
C118-H119	σ	C60-S66	σ*	9.48	0.73	0.074
C5-C6	σ	C4-C6	σ*	5.12	1.23	0.071
C68-C70	σ	C68-C69	σ*	4.02	1.28	0.064
C69-C71	σ	N96-C111	σ*	1.99	1.18	0.043
C29-C68	σ	C69-C71	σ*	1.98	1.29	0.045
C68-C69	σ	C70-H74	σ*	1.98	1.15	0.043
C28-C29	σ	C68-C70	σ*	1.88	1.3	0.044
C77-C78	σ	C78-C87	σ*	1.87	1.15	0.041
C78-C87	σ	C77-C78	σ*	1.87	1.24	0.043
C2-H49	σ	C1-C2	σ*	1.86	1.1	0.041
C33-H39	σ	C38-F67	σ*	1.84	0.83	0.035
C77-C82	σ	C78-C87	σ*	1.84	1.17	0.041
C45-H47	σ	Si40-C45	σ*	0.51	0.77	0.018
C62-C63	σ	C60-S66	σ*	0.51	0.93	0.019
C26-C27	σ	C29-S32	σ*	0.50	0.95	0.019
O90	LP(3)	N89-O91	π*	179.75	0.16	0.154
O94	LP(3)	N92-O93	π*	164.15	0.16	0.15
N96	LP(1)	C71-C76	π*	39.2	0.3	0.1
O90	LP(2)	C88-N89	σ*	14.68	0.58	0.082
O94	LP(3)	C118-H119	σ*	2.11	0.73	0.04
O105	LP(2)	C80-H107	σ*	0.54	0.75	0.018
F67	LP(1)	C33-C38	σ*	0.50	1.6	0.025

LP= lone pair, (i) donor; (j) acceptor; E(2) means energy of hyper conjugative interaction (stabilization energy); E(j) – E(i) is the energy difference between donor and acceptor i and j NBO orbitals; F(i, j) is the Fock matrix element between i and j NBO orbitals.

Table S17: Dipole polarizabilities and major contributing tensors (*esu*) of the studied compounds (**DTS(FBTTh$_2$)$_2$ R1** and **D2- D7**)

Compounds	$\alpha_{xx} \times 10^{-22}$	$\alpha_{yy} \times 10^{-22}$	$\alpha_{zz} \times 10^{-22}$	α-total $\times 10^{-22}$
DTS(FBTTh$_2$)$_2$R1	4.370	1.509	0.487	2.123
MSTD2	6.539	2.041	0.715	3.098
MSTD3	7.002	2.114	0.716	3.277
MSTD4	6.684	1.938	0.930	3.184
MSTD5	6.578	1.888	0.927	3.131
MSTD6	7.565	2.153	0.738	3.485
MSTD7	6.899	2.101	0.888	3.296

Table S18: Dipole moment and major contributing tensors (*D*) of the studied compounds **DTS(FBTTh$_2$)$_2$R1**and **D2- D7**)

Compounds	u_{xx}	u_{yy}	u_{zz}	u-total
DTS(FBTTh$_2$)$_2$R1	0.00	0.30	-0.000039	0.30
MSTD2	-2.96	4.19	-1.19	5.26
MSTD3	-4.79	3.80	0.35	6.13
MSTD4	3.74	3.33	1.41	5.20
MSTD5	3.44	-3.51	0.004	4.92
MSTD6	-8.19	2.98	0.03	8.72
MSTD7	5.50	-2.99	-1.27	6.39

Table S19: The computed hyper polarizabilities (β_{tot}) and major contributing tensors (*esu*) of the studied compounds **DTS(FBTTh$_2$)$_2$R1** and **D2-D7**)

Systems	DTS(FBTTh$_2$)$_2$R1	MSTD2	MSTD3	MSTD4	MSTD5	MSTD6	MSTD7
β_{xxx}	-5.287×10^{-33}	-6.477×10^{-27}	-8.373×10^{-27}	-7.299×10^{-27}	6.861×10^{-27}	-1.287×10^{-26}	1.00×10^{-26}
β_{xxy}	7.724×10^{-30}	1.063×10^{-27}	1.387×10^{-27}	1.341×10^{-27}	-1.241×10^{-27}	2.048×10^{-27}	-1.466×10^{-27}
β_{XYY}	1.689×10^{-33}	-1.941×10^{-28}	-2.406×10^{-28}	-2.510×10^{-28}	2.415×10^{-28}	-4.021×10^{-28}	2.654×10^{-28}
β_{yyy}	-1.668×10^{-33}	3.971×10^{-29}	5.429×10^{-29}	6.05×10^{-29}	-5.315×10^{-29}	7.164×10^{-29}	-6.046×10^{-29}
β_{xxz}	-1.403×10^{-33}	1.025×10^{-28}	3.522×10^{-29}	-1.555×10^{-28}	8.266×10^{-29}	-5.178×10^{-29}	1.813×10^{-29}
β_{yyz}	-1.193×10^{-33}	3.237×10^{-30}	7.309×10^{-31}	-3.927×10^{-30}	2.372×10^{-30}	7.044×10^{-31}	-1.483×10^{-30}
β_{xzz}	2.851×10^{-36}	-4.473×10^{-31}	2.550×10^{-30}	-3.017×10^{-30}	2.223×10^{-31}	5.535×10^{-31}	7.814×10^{-30}
β_{yzz}	8.388×10^{-31}	1.239×10^{-31}	-3.093×10^{-31}	1.403×10^{-30}	-5.82×10^{-31}	-9.303×10^{-31}	-5.895×10^{-31}
β_{zzz}	1.116×10^{-34}	6.708×10^{-31}	6.748×10^{-31}	7.772×10^{-31}	-1.01×10^{-30}	-5.115×10^{-31}	-8.630×10^{-31}
β_{total}	**8.118×10^{-30}**	**6.763×10^{-27}**	**8.730×10^{-27}**	**7.684×10^{-27}**	**7.221×10^{-27}**	**1.344×10^{-26}**	**1.039×10^{-26}**

Table S20: Second hyperpolarizability and major contributing tensor (*a.u.*) of the studied comp. **DTS(FBTTh$_2$)$_2$R1**and **D2- D7**)

Compounds	γ_x	γ_y	γ_z	<γ>
DTS(FBTTh$_2$)$_2$R1	0.396×10^{-31}	0.632×10^{-33}	0.386×10^{-35}	0.403×10^{-31}
MSTD2	1.42×10^{-31}	3.40×10^{-33}	4.35×10^{-35}	1.45×10^{-31}
MSTD3	1.97×10^{-31}	4.48×10^{-33}	1.73×10^{-35}	2.02×10^{31}
MSTD4	1.66×10^{-31}	4.67×10^{-33}	11.1×10^{-35}	1.71×10^{-31}
MSTD5	1.52×10^{-31}	4.31×10^{-33}	5.93×10^{-35}	1.57×10^{-31}
MSTD6	3.59×10^{-31}	7.22×10^{-33}	2.64×10^{-35}	3.66×10^{-31}
MSTD7	2.61×10^{-31}	6.21×10^{-33}	10.4×10^{-35}	2.67×10^{-31}

$$(\beta_x)^2 = (\beta_{xxx}+\beta_{xyy}+\beta_{xzz})^2 \quad \textbf{Eq S1}$$
$$(\beta_y)^2 = (\beta_{yyy}+\beta_{yzz}+\beta_{yxx})^2 \quad \textbf{Eq S2}$$
$$(\beta_z) = (\beta_{zzz}+\beta_{zxx}+\beta_{xyz})^2 \quad \textbf{Eq S3}$$

Table S21: Wave length, excitation energy and oscillator strength of investigated reference compound **DTS(FBTTh$_2$)$_2$R1**

NO	DFT λ (nm)	E(eV)	*f*	MO contributions
1	711.408	1.743	2.092	H→L (94%), H-1→L+1 (5%)
2	607.855	2.040	0.086	H→L+1 (92%), H-1→L (6%)
3	522.831	2.371	0.044	H-1→L (88%), H-2→L+1 (6%), H→L+1 (5%)
4	477.046	2.599	0.064	H-2→L (17%), H-1→L+1 (78%), H→L (3%)
5	439.754	2.819	0.087	H-2→L (71%), H-1→L+1 (14%), H-3→L+1 (3%), H→L+2 (9%)
6	431.099	2.876	0.727	H→L+2 (84%), H-2→L (7%), H-1→L+3 (2%)

Table S22: Wave length, excitation energy and oscillator strength of investigated compound **MSTD2**

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	810.190	1.530	1.589	H→L (83%) H-1→L (8%), H→L+1 (5%)
2	656.970	1.887	0.869	H-1→L (40%), H→L (16%), H→L+1 (28%) H-3→L (5%), H-1→L+1 (6%)
3	627.891	1.975	0.113	H-1→L (41%), H→L+1 (49%) H-1→L+1 (4%)
4	546.543	2.269	0.205	H-3→L (73%) H-4→L (7%), H-1→L (9%)
5	521.333	2.378	0.029	H→L+2 (52%), H→L+3 (25%) H-3→L (5%), H-3→L+2 (2%), H-1→L+2 (6%), H-1→L+3 (3%), H→L+1 (3%)
6	519.454	2.387	0.008	H-1→L+1 (68%), H→L+1 (11%) H-3→L+1 (6%), H→L+2 (7%)

MO=molecular orbital, HOMO=H, LUMO=L, ***f***= oscillator strength

Table S23: Wave length, excitation energy and oscillator strength of investigated compound **MSTD3**

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	859.563	1.442	1.396	H→L (87%) H-1→L (7%), H→L+1 (3%)
2	688.835	1.800	0.873	H-1→L (59%), H→L (13%), H→L+1 (15%) H-3→L (6%), H-1→L+1 (4%)
3	651.447	1.903	0.353	H-1→L (26%), H→L+1 (61%) H-1→L+1 (6%), H→L+3 (3%)
4	568.131	2.182	0.232	H-3→L (69%) H-4→L (8%), H-1→L (8%), H→L+1 (4%), H→L+2 (4%)
5	545.413	2.273	0.000	H-2→L (94%) H→L+2 (3%)
6	543.596	2.281	0.007	H→L+2 (38%), H→L+3 (28%) H-3→L (9%), H-2→L (5%), H-1→L+2 (4%), H-1→L+3 (4%), H→L+1 (7%)

MO=molecular orbital, HOMO=H, LUMO=L, ***f***= oscillator strength

Table S24: Wave length, excitation energy and oscillator strength of investigated compound **MSTD4**

No.	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	833.726	1.487	1.479	H→L (85%)H − 1→L (8%), H→L + 1 (4%)
2	672.069	1.845	0.915	H-1→L (48%), H→L (14%), H→L+1 (22%) H-3→L (5%), H-1→L+1 (5%)
3	639.815	1.938	0.188	H-1→L (35%), H→L+1 (54%) H-1→L+1 (4%), H→L+3 (2%)
4	556.478	2.228	0.223	H-3→L (69%) H-4→L (8%), H-1→L (9%), H→L+1 (3%), H→L+2 (3%)
5	534.572	2.319	0.013	H→L+2 (38%), H→L+3 (31%) H-3→L (8%), H-1→L+2 (5%), H-1→L+3 (4%), H→L+1 (7%)
6	530.819	2.336	0.001	H-2→L (98%)

Table S25: Wave length, excitation energy and oscillator strength of investigated compound **MSTD5**

No.	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	818.264	1.515	1.592	H→L (84%) H-1→L (8%), H→L+1 (4%)
2	660.540	1.877	0.917	H-1→L (36%), H→L (15%), H→L+1 (32%) H-3→L (5%), H-1→L+1 (6%)
3	631.601	1.963	0.070	H-1→L (46%), H→L+1 (45%) H-3→L (2%), H-1→L+1 (3%)
4	548.405	2.260	0.205	H-3→L (65%), H-1→L (10%) H-4→L (7%), H→L+1 (3%), H→L+2 (6%)
5	531.296	2.337	0.036	H-3→L (12%), H→L+2 (44%), H→L+3 (26%) H-1→L+2 (5%), H-1→L+3 (3%), H→L+1 (5%)
6	522.673	2.372	0.018	H-1→L+1 (67%) H-3→L+1 (7%), H→L+1 (9%), H→L+2 (9%)

Table S26: Wave length, excitation energy and oscillator strength of investigated compound **MSTD6**

No.	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	982.747	1.262	0.841	H→L (92%) H-1→L (5%)
2	780.997	1.588	1.228	H-1→L (27%), H→L+1 (52%) H-1→L+1 (6%), H→L (6%), H→L+2 (4%)
3	760.074	1.631	0.024	H-1→L (61%), H→L+1 (32%) H-3→L (2%)
4	637.348	1.945	0.717	H-3→L (10%), H-1→L+1 (29%), H→L+1 (12%), H→L+2 (30%) H-3→L+1 (3%), H-1→L (4%), H-1→L+2 (7%)
5	617.816	2.007	0.035	H-3→L (31%), H-1→L+1 (44%) H-4→L (5%), H-2→L (2%), H-1→L (2%), H→L+2 (8%)
6	609.494	2.034	0.003	H-2→L (97%)

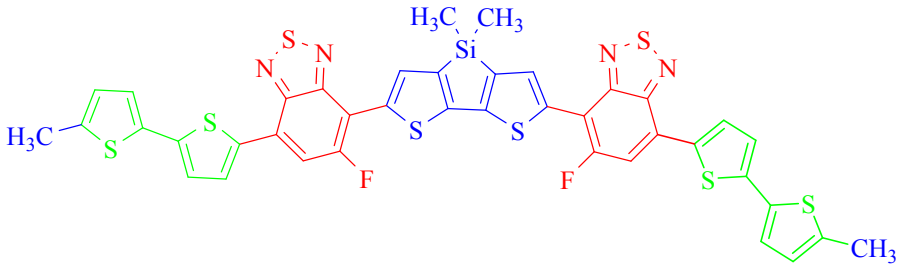
MO=molecular orbital, HOMO=H, LUMO=L, f= oscillator strength

Table S27: Wave length, excitation energy and oscillator strength of investigated compound **MSTD7**

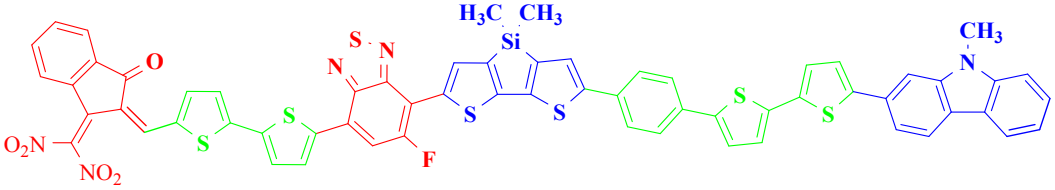
No.	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	930.247	1.333	1.009	H→L (91%) H-1→L (5%)
2	732.243	1.693	0.704	H-1→L (75%) H-3→L (6%), H-1→L+1 (2%), H→L (8%), H→L+1 (7%)
3	676.617	1.832	0.801	H-1→L (14%), H→L+1 (71%) H-1→L+1 (8%), H→L+3 (3%)

4	596.791	2.078	0.140	H-3→L (77%) H-4→L (8%), H-1→L (6%), H→L+1 (4%)
5	580.881	2.134	0.002	H-2→L (98%)
6	546.351	2.269	0.035	H-1→L+1 (34%), H→L+1 (15%), H→L+3 (29%) H-3→L (2%), H-3→L+1 (2%), H-1→L+3 (6%), H→L+2 (9%)

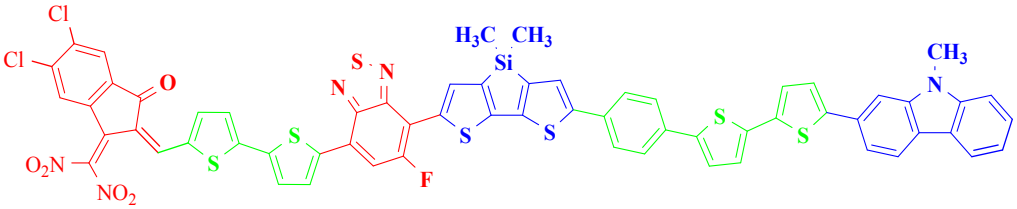
DTS(FBTTh$_2$)$_2$R1



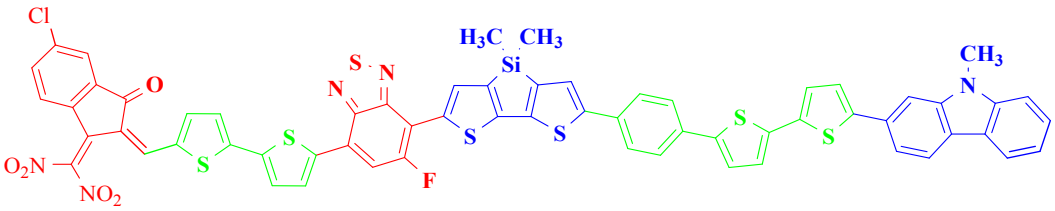
MSTD2



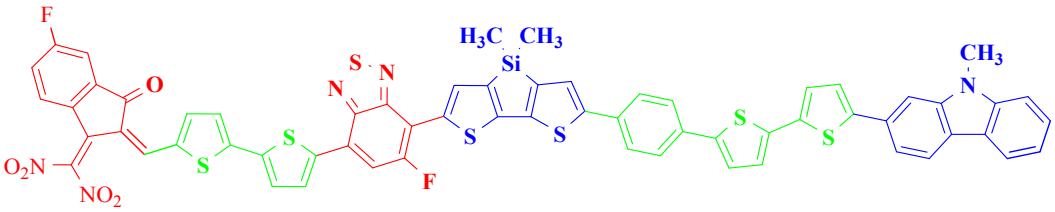
MSTD3



MSTD4



MSTD5



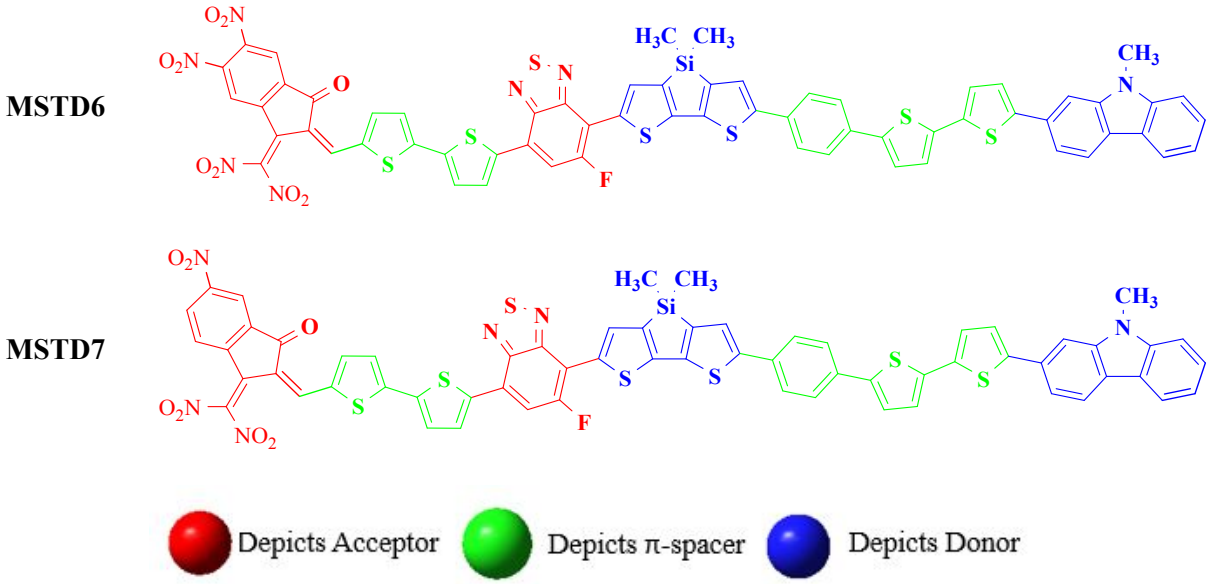
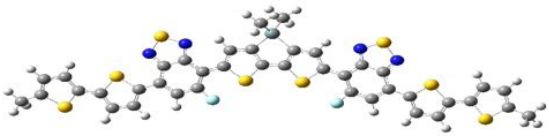
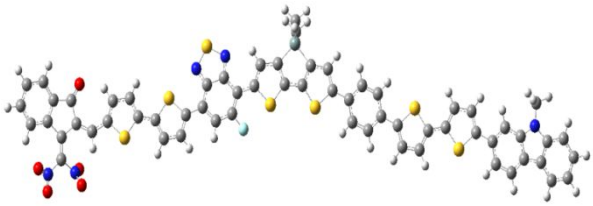


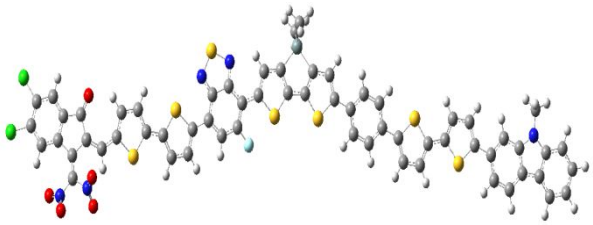
Figure S1: The structures of **DTS(FBTTh$_2$)$_2$R1** and its derivatives



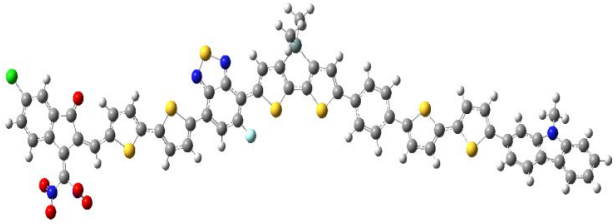
DTS(FBTTh$_2$)$_2$R1



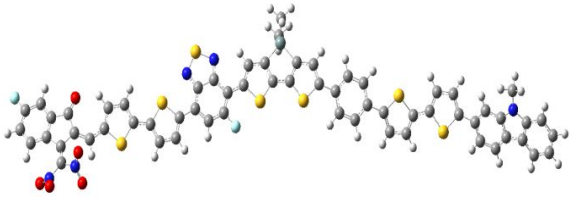
MSTD2



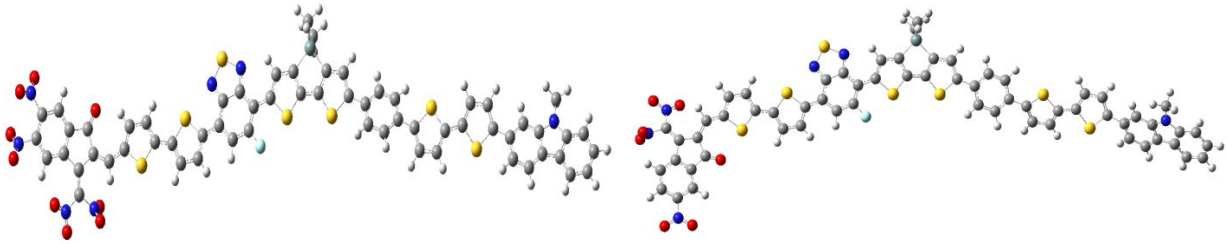
MSTD3



MSTD4



MSTD5



MSTD6 **MSTD7**

Figure S2: The optimized structures of **DTS(FBTTh$_2$)$_2$R1**and its derivatives