

## Supporting Information

### ***Optoelectronic properties of oligomers based on tetrazine, benzothiadiazole, benzodithiophene and thiophene moieties, for photovoltaic application. A theoretical study.***

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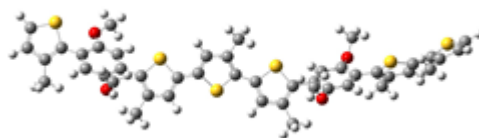
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#### **List of the supporting information:**

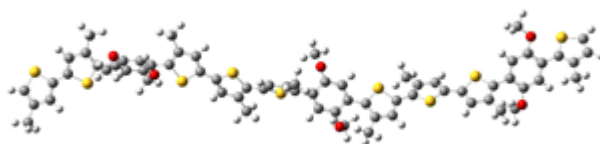
1. **Table S1.** Optimized geometry (cartesian coordinates in Å) of the A-G oligomers at the B3LYP/6-311G(d,p) level.
2. **Figure S1:** Plots of the simulated absorption spectra, calculated at the TD-B3LYP/6-311G(d,p) level for the A-G oligomers.

**Table S1:** Optimized geometry (cartesian coordinates in Å) of the A-G oligomers at the B3LYP/6-311G(d,p) level.

**1) A1<sub>1</sub>**



1	C	-13.2796	-0.4734	1.4800	34	C	10.0030	-1.5294	-0.5929	67	H	15.3433	-3.1249	0.5937
2	C	-12.6395	-1.0657	0.4094	35	C	11.0538	-0.7269	-0.0874	68	H	-13.5706	1.2987	2.6545
3	S	-13.6167	-2.3592	-0.2667	36	C	10.7134	0.5293	0.4203	69	H	-12.1888	0.3317	3.1665
4	C	-14.8790	-2.0741	0.8792	37	C	8.6969	-1.0488	-0.6048	70	H	-9.8941	-0.0412	-3.8991
5	C	-14.5567	-1.0624	1.7338	38	C	8.3706	0.2296	-0.1173	71	H	-8.2628	0.2541	-3.2788
6	C	-9.6536	-0.5153	-1.8201	39	C	9.4068	1.0112	0.4158	72	H	-3.6576	4.2335	-0.0451
7	C	-8.9143	-0.3134	-0.6746	40	O	10.3576	-2.7553	-1.0680	73	H	-2.7718	4.1230	-1.5739
8	S	-9.9175	-0.4616	0.7555	41	O	9.1747	2.2687	0.9343	74	H	0.9752	-1.4570	3.1019
9	C	-11.3492	-0.7804	-0.1994	42	C	14.7894	-1.1615	-0.2345	75	H	-0.5309	-0.6246	2.6992
10	C	-11.0242	-0.7815	-1.5341	43	C	14.6010	-2.3880	0.3274	76	H	6.6866	3.4103	-2.1607
11	C	-5.1380	-0.3749	-0.9917	44	S	12.9247	-2.7268	0.5662	77	H	7.5522	3.7326	-0.6489
12	C	-4.7446	0.7450	-0.2457	45	C	12.4605	-1.1645	-0.0837	78	H	13.8366	1.7007	-0.4036
13	C	-5.7582	1.4782	0.4034	46	C	13.5737	-0.4475	-0.4734	79	H	14.2907	0.9538	-1.9320
14	C	-6.4716	-0.7450	-1.1245	47	C	-12.7477	0.6786	2.2907	80	H	-7.2429	-3.8162	-1.9088
15	C	-7.4890	0.0205	-0.5204	48	C	-9.1215	-0.4166	-3.2236	81	H	-7.9635	-2.9107	-0.5535
16	C	-7.0933	1.1209	0.2528	49	C	-3.4102	3.5713	-0.8791	82	H	9.3639	1.7915	2.9590
17	O	-6.7614	-1.8463	-1.8995	50	C	0.3352	-1.1375	2.2766	83	H	8.5580	3.3291	2.5502
18	O	-5.4704	2.5902	1.1643	51	C	7.2657	2.9498	-1.3563	84	H	9.8650	-4.5257	-1.8803
19	C	-1.3057	2.2735	-0.1838	52	C	13.5632	0.9149	-1.1165	85	H	8.5986	-3.8528	-0.8220
20	C	-0.8256	1.0506	0.2248	53	C	-7.0666	-3.0381	-1.1667	86	H	-4.8207	3.2742	2.9596
21	S	-2.1512	-0.0902	0.3384	54	C	8.6650	2.2809	2.2714	87	H	-5.7109	1.7315	3.0522
22	C	-3.3238	1.1190	-0.1504	55	C	9.3499	-3.6142	-1.5827	88	H	-12.0795	1.3116	1.7051
23	C	-2.7116	2.3276	-0.4022	56	C	-4.9776	2.3092	2.4785	89	H	-8.7888	-1.3909	-3.5915
24	C	2.5251	-0.2737	1.2662	57	H	-15.7801	-2.6670	0.8503	90	H	-4.3451	3.3339	-1.3878
25	C	3.0772	0.6122	0.3719	58	H	-15.2143	-0.7229	2.5244	91	H	-0.0311	-2.0410	1.7780
26	S	1.8104	1.4899	-0.4546	59	H	-11.7664	-0.9355	-2.3077	92	H	8.1879	2.5515	-1.7811
27	C	0.5542	0.6735	0.4652	60	H	-4.3941	-0.9670	-1.5113	93	H	12.5838	1.1649	-1.5250
28	C	1.1052	-0.2542	1.3311	61	H	-7.8407	1.7395	0.7351	94	H	-6.2237	-3.3282	-0.5296
29	C	6.4624	1.8721	-0.6819	62	H	-0.6588	3.1308	-0.3239	95	H	7.6896	1.7882	2.3304
30	C	6.9785	0.7041	-0.1641	63	H	4.4683	2.7967	-0.8763	96	H	8.8568	-3.1751	-2.4568
31	S	5.7040	-0.3135	0.4875	64	H	11.4808	1.1572	0.8550	97	H	-4.0301	1.7637	2.4402
32	C	4.4710	0.8582	0.0743	65	H	7.9033	-1.6465	-1.0310	98	H	3.1281	-0.9124	1.9001
33	C	5.0469	1.9463	-0.5363	66	H	15.7654	-0.7674	-0.4894					

2)  $A_{1g}$ 

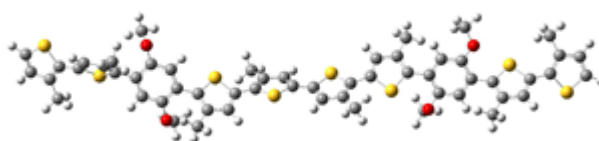
1	C	3.0191	0.5628	-2.4929	41	C	24.9728	6.9546	-2.1666	81	C	24.1267	3.5280	1.3075
2	C	3.3570	-0.0598	-1.3162	42	C	24.8017	4.5881	-0.6993	82	C	37.4374	14.0160	0.7098
3	S	1.9094	-0.5069	-0.4337	43	C	23.6838	5.0059	-1.4490	83	C	39.0493	8.8477	5.2636
4	C	0.8945	0.1374	-1.6849	44	C	23.8000	6.2078	-2.1617	84	C	24.8548	9.3189	-2.1628
5	C	1.6127	0.6817	-2.7126	45	O	24.7795	3.4241	0.0373	85	H	4.3362	-2.0043	0.5625
6	C	6.4338	-1.3255	0.4473	46	O	24.9995	8.1105	-2.9161	86	H	11.6420	-1.4342	-0.4921
7	C	7.1375	-0.3616	-0.2412	47	C	29.3112	8.3653	-2.1364	87	H	8.2245	2.0402	0.1839
8	S	6.0702	0.5825	-1.2685	48	C	29.4857	8.4555	-0.7746	88	H	15.9353	0.3466	0.9410
9	C	4.6727	-0.3499	-0.7810	49	S	28.1519	7.6631	0.0401	89	H	1.3249	0.8023	-4.8463
10	C	5.0445	-1.3093	0.1278	50	C	27.3818	7.2460	-1.4794	90	H	-0.0819	1.2922	-3.8959
11	C	10.3319	1.6414	0.0798	51	C	28.1312	7.6842	-2.5497	91	H	6.3036	-2.4946	2.2415
12	C	11.3347	0.6531	-0.0722	52	C	31.9956	10.0984	1.4766	92	H	7.3055	-3.2260	0.9763
13	C	10.9098	-0.6554	-0.3223	53	C	32.9377	9.8222	0.5145	93	H	13.7314	-1.9095	1.0397
14	C	8.9865	1.2911	0.0205	54	S	32.1970	8.9564	-0.8121	94	H	14.1720	-0.9291	2.4344
15	C	8.5713	-0.0343	-0.2011	55	C	30.6102	9.0278	-0.0588	95	H	9.7185	-2.3678	-2.6743
16	C	9.5648	-1.0073	-0.3915	56	C	30.6792	9.6570	1.1711	96	H	8.6962	-3.6851	-2.0412
17	O	10.7686	2.9119	0.3030	57	C	36.5552	10.5376	-0.2327	97	H	10.3945	4.8610	0.6175
18	O	9.2504	-2.3276	-0.6389	58	C	36.7163	10.7586	1.1181	98	H	9.1842	4.0638	-0.4202
19	C	15.0513	0.7613	0.4720	59	S	35.2042	10.5201	1.9796	99	H	1.3168	2.3640	-4.0283
20	C	15.0910	1.8764	-0.3301	60	C	34.3484	10.1411	0.5006	100	H	7.926489	-1.87196	1.904195
21	S	13.4783	2.2998	-0.8499	61	C	35.2132	10.1947	-0.5660	101	H	12.48463	-1.01909	1.91516
22	C	12.7719	0.9507	0.0223	62	C	39.4425	10.6583	3.7403	102	H	7.996976	-2.06542	-2.2959
23	C	13.7498	0.2253	0.6767	63	C	40.2754	11.7385	3.3621	103	H	9.181621	3.778547	1.345424
24	C	1.0086	1.3180	-3.9343	64	C	39.8785	12.4973	2.2582	104	H	3.760878	0.908727	-3.20238
25	C	7.0240	-2.2807	1.4479	65	C	38.2997	10.3621	3.0031	105	H	15.37799	4.555853	-1.33281
26	C	13.5148	-0.9710	1.5618	66	C	37.9253	11.1162	1.8764	106	H	20.4963	1.552398	-1.99266
27	C	8.8946	-2.6144	-1.9953	67	C	38.7315	12.2089	1.5230	107	H	26.82853	4.939549	-0.16653
28	C	9.8147	3.9518	0.4685	68	O	39.8413	9.9440	4.8288	108	H	22.96753	6.567601	-2.7544
29	C	17.5710	4.4470	-1.5090	69	O	38.4273	13.0167	0.4463	109	H	30.02013	8.786195	-2.83884
30	C	18.5565	3.5106	-1.2540	70	C	43.7020	12.7595	4.5363	110	H	34.89641	9.994928	-1.58251
31	S	17.8565	2.0224	-0.6323	71	C	43.1961	12.7554	5.8012	111	H	40.46433	13.35784	1.96107
32	C	16.2345	2.6701	-0.7236	72	S	41.5420	12.2600	5.8224	112	H	37.69041	9.509153	3.267477
33	C	16.2717	3.9580	-1.2034	73	C	41.5178	12.0773	4.0774	113	H	44.72901	13.01545	4.307081
34	C	22.2305	2.9007	-1.7896	74	C	42.7528	12.3763	3.5380	114	H	43.70094	12.98903	6.72613
35	C	22.4343	4.2296	-1.4845	75	C	17.7974	5.8298	-2.0605	115	H	16.90261	6.181097	-2.57909
36	S	20.9158	5.0359	-1.1407	76	C	23.3074	1.9270	-2.1829	116	H	18.02017	6.550919	-1.26697
37	C	19.9955	3.5724	-1.4257	77	C	27.7865	7.4640	-3.9972	117	H	22.92224	1.204534	-2.90682
38	C	20.8524	2.5458	-1.7491	78	C	29.5173	9.9019	2.0970	118	H	24.16295	2.436072	-2.62863
39	C	25.9813	5.3236	-0.7220	79	C	37.6522	10.6099	-1.2589	119	H	27.23031	8.311344	-4.40685
40	C	26.1079	6.5085	-1.4607	80	C	43.1215	12.2876	2.0800	120	H	28.69567	7.333024	-4.5894

continues

### A<sub>1</sub> geometry continuation

121	H	29.72924	10.74746	2.754936	130	H	37.31864	14.58255	-0.21368	139	H	38.62674	10.40325	-0.8146
122	H	28.59949	10.12174	1.548359	131	H	39.55361	8.45203	6.143417	140	H	42.41778	11.67188	1.519381
123	H	37.47655	9.88371	-2.05659	132	H	38.03746	9.166124	5.536886	141	H	24.62393	4.272394	1.939231
124	H	37.71138	11.60518	-1.70724	133	H	24.87666	10.13466	-2.88496	142	H	36.4793	13.56422	0.984597
125	H	43.14743	13.27613	1.608113	134	H	23.89792	9.33133	-1.62905	143	H	38.99121	8.066563	4.497727
126	H	44.11805	11.85174	1.96772	135	H	18.62912	5.853498	-2.76688	144	H	25.67412	9.443913	-1.44851
127	H	24.20704	2.546481	1.773808	136	H	23.68033	1.376357	-1.31521	145	H	32.23167	10.64376	2.382224
128	H	23.07093	3.790752	1.192775	137	H	27.16204	6.57935	-4.12813	146	H	-0.17863	0.077105	-1.5833
129	H	37.76664	14.689	1.509397	138	H	29.31775	9.03376	2.733936					

### 3) A<sub>2</sub>



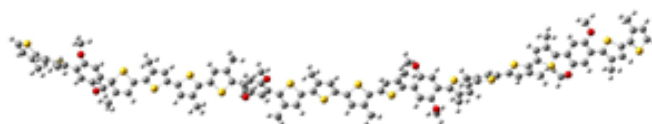
1	C	2.2604	3.6446	2.5603	29	C	19.2558	8.7398	-6.6396	57	S	27.7701	8.5688	-14.4325
2	C	2.2520	4.6029	1.5659	30	C	19.3025	7.8890	-7.7310	58	C	27.3275	9.1350	-12.8342
3	S	0.6318	4.8255	0.9251	31	S	17.9739	6.7366	-7.6775	59	C	28.3758	9.8178	-12.2494
4	C	-0.0160	3.6491	2.0133	32	C	17.3562	7.4166	-6.1885	60	C	28.3442	10.4848	-10.8991
5	C	0.9570	3.1111	2.8018	33	C	18.1579	8.4581	-5.7835	61	C	24.7347	6.0595	-8.9299
6	C	4.5074	7.2220	0.0689	34	C	3.4690	3.2059	3.3439	62	C	23.6959	9.8076	-14.9056
7	C	5.4892	6.2563	0.0153	35	C	11.9716	8.0768	0.2244	63	C	31.4808	9.0074	-17.4080
8	S	4.9069	4.7312	0.6545	36	C	13.5286	4.2285	-5.1366	64	C	32.5309	8.7925	-16.5664
9	C	3.3322	5.4057	1.0136	37	C	20.2241	9.8573	-6.3554	65	S	32.0255	8.7947	-14.9132
10	C	3.2960	6.7247	0.6312	38	C	5.5629	6.2444	-3.3211	66	C	30.3596	9.1174	-15.3677
11	C	8.5355	6.9735	-2.1219	39	C	10.8185	4.3451	0.5541	67	C	30.2310	9.1955	-16.7404
12	C	9.5968	6.5865	-1.2917	40	C	4.6774	8.6557	-0.3533	68	C	28.9534	9.4757	-17.4865
13	C	9.2686	6.0351	-0.0369	41	C	21.0980	7.3219	-10.9795	69	H	-1.0724	3.4294	2.0063
14	C	7.2071	6.8554	-1.7289	42	C	22.2199	7.8818	-10.3953	70	H	0.7597	2.3585	3.5551
15	C	6.8813	6.3545	-0.4527	43	S	21.8884	8.3468	-8.7371	71	H	2.4213	7.3450	0.7837
16	C	7.9411	5.9369	0.3646	44	C	20.2204	7.8274	-8.8506	72	H	8.7397	7.4066	-3.0938
17	O	6.2338	7.2861	-2.6035	45	C	19.9830	7.2983	-10.0995	73	H	7.7387	5.5468	1.3549
18	O	10.2414	5.6219	0.8468	46	C	21.0154	6.7581	-12.3747	74	H	14.1758	7.7552	-1.5426
19	C	13.2412	7.3222	-1.8779	47	C	24.7955	9.0199	-12.9235	75	H	15.8434	5.0009	-6.5640
20	C	13.1263	6.6674	-3.0824	48	C	26.0189	8.8046	-12.2467	76	H	17.9680	9.0212	-4.8780
21	S	11.4790	6.1069	-3.2898	49	C	25.9492	8.2682	-10.9577	77	H	3.1775	2.9002	4.3516
22	C	10.9910	6.7538	-1.7345	50	C	23.5859	8.7186	-12.3035	78	H	3.9659	2.3502	2.8744
23	C	12.0455	7.3810	-1.1070	51	C	23.5255	8.1772	-11.0059	79	H	4.0652	9.3122	0.2700
24	C	15.5027	5.7112	-5.8205	52	C	24.7421	7.9640	-10.3381	80	H	5.7169	8.9761	-0.2701
25	C	16.1671	6.8879	-5.5631	53	O	24.8863	9.5507	-14.1757	81	H	12.2787	7.4130	1.0370
26	S	15.3460	7.7675	-4.2930	54	O	24.7710	7.4859	-9.0437	82	H	12.6260	8.9522	0.2334
27	C	14.1419	6.5008	-4.1045	55	C	29.5192	9.8820	-13.0951	83	H	14.1182	3.4253	-5.5839
28	C	14.3594	5.4778	-5.0101	56	C	29.3695	9.2612	-14.3111	84	H	13.1650	3.8821	-4.1674

continues

## A2<sub>1</sub> geometry continuation

85	H	19.7852	10.5673	-5.6516	97	H	28.8705	9.8911	-10.1437	109	H	20.4929	10.4024	-7.2626
86	H	21.1535	9.4861	-5.9114	98	H	28.8398	11.4583	-10.9458	110	H	6.2743	5.6665	-3.9214
87	H	4.8505	6.7381	-3.9815	99	H	24.7689	5.8343	-7.8644	111	H	11.3284	4.3512	-0.4137
88	H	5.0259	5.5746	-2.6429	100	H	23.8141	5.6505	-9.3587	112	H	4.3819	8.8000	-1.3959
89	H	11.5430	4.1482	1.3439	101	H	24.0195	10.2087	-15.8645	113	H	20.3987	5.8556	-12.3801
90	H	10.0518	3.5623	0.5604	102	H	23.1200	8.8906	-15.0723	114	H	27.3243	10.6403	-10.5467
91	H	19.0183	6.9008	-10.3902	103	H	31.5841	9.0482	-18.4853	115	H	25.6004	5.6085	-9.4275
92	H	20.5531	7.4659	-13.0719	104	H	33.5692	8.6350	-16.8148	116	H	23.0657	10.5470	-14.3992
93	H	21.9991	6.4983	-12.7669	105	H	28.2632	10.0793	-16.8954	117	H	29.1662	10.0117	-18.4148
94	H	26.8620	8.0686	-10.4108	106	H	4.2066	4.0050	3.4323	118	H	28.4322	8.5507	-17.7556
95	H	22.6568	8.9403	-12.8068	107	H	10.9559	8.4060	0.4468					
96	H	30.4254	10.4082	-12.8213	108	H	12.6542	4.3880	-5.7763					

## 4) A2<sub>2</sub>



1	C	-34.7084	6.9874	-0.4495	28	C	-21.1405	2.1849	-0.0262	55	C	-5.0506	-5.0107	-1.1808
2	C	-34.3877	6.0431	0.5056	29	C	-16.8751	-2.0368	-1.1310	56	C	-4.5044	-4.7239	0.0490
3	S	-35.4253	6.1998	1.9142	30	C	-16.1245	-1.3474	-0.1954	57	S	-5.7240	-4.0282	1.0906
4	C	-36.2893	7.5131	1.1955	31	S	-17.0404	-0.0011	0.4693	58	C	-6.9512	-4.1353	-0.1560
5	C	-35.7962	7.8181	-0.0380	32	C	-18.4355	-0.3793	-0.5157	59	C	-6.4278	-4.6831	-1.3120
6	C	-32.2889	2.9396	0.8938	33	C	-18.1707	-1.4778	-1.2995	60	C	-7.1983	-4.9743	-2.5735
7	C	-31.2486	3.6483	0.3330	34	C	-34.0407	7.1389	-1.7905	61	C	-10.6105	-0.0886	-1.5784
8	S	-31.7456	5.2806	-0.0711	35	C	-26.4057	0.3751	-3.0143	62	C	-9.2067	-5.0888	3.3011
9	C	-33.3745	4.9989	0.5040	36	C	-21.5049	3.5668	0.4481	63	C	-1.1737	-5.3322	1.6612
10	C	-33.4796	3.7172	0.9866	37	C	-16.4214	-3.2512	-1.8970	64	C	-0.6120	-5.1031	0.4269
11	C	-27.7673	2.1845	0.6512	38	C	-29.4247	3.5650	3.1290	65	S	-1.8609	-4.7024	-0.7302
12	C	-27.2480	2.3318	-0.6427	39	C	-26.7476	4.2820	-3.0718	66	C	-3.1284	-4.9030	0.4707
13	C	-28.0609	2.9767	-1.5962	40	C	-32.2279	1.4969	1.3150	67	C	-2.5898	-5.2224	1.7048
14	C	-29.0427	2.6216	0.9910	41	C	-12.8975	-1.5561	1.7161	68	C	-3.3752	-5.4755	2.9644
15	C	-29.8761	3.2165	0.0227	42	C	-12.3189	-2.0740	0.5726	69	H	-37.1077	7.9764	1.7246
16	C	-29.3445	3.3938	-1.2625	43	S	-13.4949	-2.1864	-0.7228	70	H	-36.2012	8.6075	-0.6589
17	O	-29.4754	2.4118	2.2819	44	C	-14.7787	-1.5737	0.2969	71	H	-34.4112	3.3213	1.3721
18	O	-27.6346	3.1730	-2.8917	45	C	-14.2813	-1.2774	1.5450	72	H	-27.1800	1.6915	1.4167
19	C	-24.0943	0.7572	-1.9610	46	C	-12.1850	-1.2749	3.0140	73	H	-29.9490	3.8449	-2.0401
20	C	-23.4158	1.3842	-0.9411	47	C	-9.0733	-3.9094	1.2151	74	H	-23.5935	0.1306	-2.6888
21	S	-24.5452	2.3035	0.0342	48	C	-8.3065	-3.6073	0.0650	75	H	-18.9970	2.2626	0.4698
22	C	-25.9026	1.8323	-0.9711	49	C	-8.8944	-2.7763	-0.8939	76	H	-18.8933	-1.8820	-1.9978
23	C	-25.4970	0.9976	-1.9900	50	C	-10.3635	-3.4046	1.3524	77	H	-34.7547	7.5090	-2.5303
24	C	-19.8158	1.6794	0.0665	51	C	-10.9472	-2.5724	0.3801	78	H	-33.2123	7.8543	-1.7506
25	C	-19.6417	0.4118	-0.4375	52	C	-10.1827	-2.2707	-0.7580	79	H	-33.1916	1.0096	1.1473
26	S	-21.1680	-0.2097	-1.0235	53	O	-8.4831	-4.7239	2.1351	80	H	-31.4657	0.9499	0.7584
27	C	-22.0055	1.2821	-0.6193	54	O	-10.6938	-1.5026	-1.7840	81	H	-26.4567	0.9824	-3.9220

continues

## A<sub>2</sub> geometry continuation

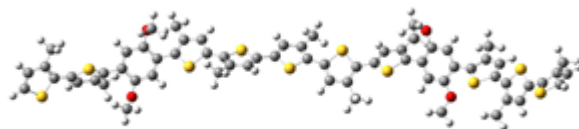
82	H	-26.0457	-0.6198	-3.2882	127	C	5.1993	-5.6381	1.6283	172	C	33.2510	4.1886	-0.8705
83	H	-20.6149	4.1979	0.4940	128	C	10.6939	-3.4930	1.0922	173	C	33.2433	5.4105	-0.2435
84	H	-22.2265	4.0474	-0.2154	129	C	11.3298	-3.9321	-0.0777	174	S	31.6483	5.7468	0.3848
85	H	-17.2836	-3.8409	-2.2157	130	C	10.5456	-4.6336	-1.0153	175	C	31.0168	4.2236	-0.2090
86	H	-15.8615	-2.9758	-2.7968	131	C	9.3531	-3.7560	1.3492	176	C	32.0012	3.5070	-0.8609
87	H	-29.7737	3.2404	4.1088	132	C	8.5835	-4.5050	0.4363	177	C	31.8375	2.1346	-1.4604
88	H	-30.0753	4.3620	2.7568	133	C	9.2108	-4.9160	-0.7485	178	C	26.1286	3.5621	-2.9357
89	H	-26.5169	4.3198	-4.1361	134	O	8.8210	-3.3028	2.5363	179	C	29.0149	4.4864	3.5139
90	H	-27.2308	5.2182	-2.7709	135	O	11.0810	-5.0988	-2.1966	180	C	35.8894	7.9319	0.6245
91	H	-14.9000	-0.8729	2.3366	136	C	15.0292	-3.8429	-0.7621	181	C	36.3648	7.7350	-0.6374
92	H	-12.3762	-2.0563	3.7580	137	C	14.9853	-2.4850	-0.5423	182	S	35.3984	6.5938	-1.5049
93	H	-11.1058	-1.2021	2.8771	138	S	13.3454	-2.0100	-0.1456	183	C	34.3405	6.3589	-0.1224
94	H	-8.3352	-2.4980	-1.7778	139	C	12.7577	-3.6548	-0.3032	184	C	34.7323	7.1532	0.9370
95	H	-10.9613	-3.6838	2.2074	140	C	13.7828	-4.5169	-0.6282	185	C	34.0699	7.2009	2.2884
96	H	-4.4822	-5.4849	-1.9713	141	C	17.4609	0.3238	-0.7546	186	H	0.7116	-5.4445	-2.1013
97	H	-7.0247	-4.2097	-3.3385	142	C	18.4243	-0.5894	-0.3954	187	H	4.5842	-6.1318	2.3705
98	H	-6.8818	-5.9311	-2.9971	143	S	17.6888	-2.1521	-0.1197	188	H	11.2572	-2.9528	1.8437
99	H	-11.0345	0.3769	-2.4676	144	C	16.0933	-1.5498	-0.5466	189	H	8.6598	-5.4962	-1.4789
100	H	-11.1845	0.2194	-0.6987	145	C	16.1426	-0.1989	-0.8435	190	H	15.9465	-4.3572	-1.0213
101	H	-8.5367	-5.7261	3.8756	146	C	22.1589	-0.8149	-0.0319	191	H	17.6952	1.3550	-0.9886
102	H	-9.4742	-4.2114	3.9002	147	C	22.1600	0.5625	0.0958	192	H	20.6581	-2.3954	-0.3464
103	H	-0.5839	-5.6152	2.5244	148	S	20.5253	1.2009	-0.0198	193	H	2.8827	-6.0433	-3.2734
104	H	-4.3298	-5.9619	2.7560	149	C	19.8470	-0.3970	-0.2348	194	H	3.8148	-4.5773	-2.9763
105	H	-33.6385	6.1915	-2.1521	150	C	20.8504	-1.3372	-0.2187	195	H	6.8785	-6.8368	3.4064
106	H	-27.4247	0.2789	-2.6373	151	C	3.5061	-5.5316	-2.5370	196	H	8.3873	-6.1676	2.7669
107	H	-21.9447	3.5476	1.4507	152	C	13.6427	-6.0044	-0.8024	197	H	13.4819	-6.2684	-1.8510
108	H	-15.7755	-3.8928	-1.2951	153	C	14.9703	0.6526	-1.2531	198	H	14.5448	-6.5147	-0.4557
109	H	-28.3982	3.9387	3.2142	154	C	23.3741	-1.7021	0.0272	199	H	15.3156	1.5383	-1.7904
110	H	-25.8221	4.1483	-2.5039	155	C	8.0292	-2.1148	2.4259	200	H	14.2808	0.1102	-1.9031
111	H	-31.9775	1.4034	2.3751	156	C	11.2095	-4.1138	-3.2273	201	H	23.0913	-2.7104	0.3374
112	H	-12.5376	-0.3328	3.4421	157	C	7.3480	-5.9359	3.0035	202	H	23.8627	-1.7841	-0.9492
113	H	-8.2722	-5.0225	-2.3917	158	C	24.4235	3.4287	0.9759	203	H	7.6989	-1.8723	3.4355
114	H	-9.5672	0.2254	-1.4628	159	C	25.4269	2.7740	0.2868	204	H	7.1561	-2.2758	1.7865
115	H	-10.1136	-5.6502	3.0511	160	S	24.8400	1.2617	-0.3778	205	H	11.6256	-4.6287	-4.0929
116	H	-2.8070	-6.1166	3.6420	161	C	23.2496	1.4954	0.3142	206	H	10.2311	-3.6955	-3.4886
117	H	-3.5921	-4.5446	3.4986	162	C	23.2034	2.6982	0.9806	207	H	22.3091	3.0536	1.4776
118	C	2.7417	-5.3318	-1.2551	163	C	24.5465	4.7745	1.6427	208	H	24.6721	4.6787	2.7270
119	C	3.3019	-5.1909	0.0023	164	C	28.9058	3.9686	1.1735	209	H	25.3943	5.3421	1.2580
120	S	2.0531	-4.9901	1.2230	165	C	29.5929	3.8819	-0.0600	210	H	29.3445	3.3776	-2.1358
121	C	0.7779	-5.1508	0.0370	166	C	28.8645	3.4372	-1.1674	211	H	27.0621	3.6224	2.2140
122	C	1.3215	-5.3081	-1.2167	167	C	27.5649	3.6035	1.2583	212	H	34.1488	3.7662	-1.3048
123	C	6.6013	-5.4530	1.7903	168	C	26.8413	3.1550	0.1385	213	H	31.7338	2.1801	-2.5500
124	C	7.1750	-4.8421	0.6955	169	C	27.5249	3.0721	-1.0847	214	H	32.7166	1.5208	-1.2462
125	S	5.9722	-4.4919	-0.5315	170	O	29.6370	4.3981	2.2408	215	H	25.7207	3.0477	-3.8052
126	C	4.6865	-5.1890	0.4329	171	O	26.9064	2.5955	-2.2223	216	H	25.3069	3.9428	-2.3207

continues

## A<sub>2</sub> geometry continuation

217	H	29.7832	4.8538	4.1920	223	H	12.7920	-6.3933	-0.2415	229	H	23.6402	5.3629	1.4766
218	H	28.1746	5.1896	3.5039	224	H	14.3983	0.9981	-0.3856	230	H	30.9608	1.6206	-1.0656
219	H	36.3543	8.6053	1.3340	225	H	24.1171	-1.3261	0.7327	231	H	26.7561	4.3976	-3.2654
220	H	37.2230	8.1875	-1.1099	226	H	8.6265	-1.2861	2.0299	232	H	28.6664	3.5068	3.8593
221	H	33.5821	6.2565	2.5337	227	H	11.8840	-3.3069	-2.9255	233	H	34.8080	7.4154	3.0652
222	H	4.4074	-6.1278	-2.3834	228	H	7.3615	-5.1761	3.7893	234	H	33.3077	7.9861	2.3363

## 5) A<sub>3</sub><sub>1</sub>



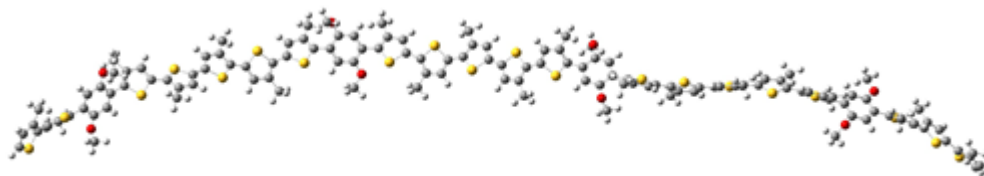
1	C	-11.6507	-4.7027	9.5069	33	C	2.7292	2.5926	0.2481	65	C	14.2796	3.8108	-11.5636
2	C	-11.8531	-3.5806	8.7279	34	C	-10.3197	-5.1846	10.0200	66	C	14.9072	4.7336	-10.5514
3	S	-13.5592	-3.3670	8.3690	35	C	-9.9312	0.9319	7.3379	67	C	11.8909	1.7986	-6.1782
4	C	-13.9805	-4.7705	9.2857	36	C	-2.6137	0.7811	6.7565	68	C	8.9079	4.1538	-12.1453
5	C	-12.8766	-5.3696	9.8151	37	C	-1.7909	-1.7825	0.5181	69	C	14.7946	1.2335	-17.0359
6	C	-9.9717	-0.5648	7.4816	38	C	4.7336	4.1085	-0.2440	70	C	16.1125	1.0668	-16.6815
7	C	-8.9688	-1.4276	7.0956	39	C	-9.3993	-0.7882	3.8444	71	S	16.3428	1.5646	-15.0204
8	S	-9.3788	-3.0858	7.4917	40	C	-3.5543	-3.0215	6.4862	72	C	14.6605	2.0371	-14.8552
9	C	-10.9069	-2.6095	8.2001	41	C	4.7933	2.9890	-5.4544	73	C	13.9620	1.7794	-16.0207
10	C	-11.0592	-1.2481	8.0994	42	C	6.0376	3.2730	-4.9190	74	C	12.5023	2.0701	-16.2501
11	C	-6.3196	-0.0862	4.7406	43	S	5.9946	3.1897	-3.1664	75	C	19.2260	0.0213	-18.5016
12	C	-5.1280	-0.5479	5.3171	44	C	4.2832	2.8189	-3.1552	76	C	18.4498	-0.9243	-19.1024
13	C	-5.2361	-1.3551	6.4671	45	C	3.8218	2.7368	-4.4504	77	S	16.8186	-0.8565	-18.5344
14	C	-7.5658	-0.3764	5.2848	46	C	4.4524	2.9833	-6.9211	78	C	17.1871	0.4983	-17.4781
15	C	-7.6703	-1.1385	6.4656	47	C	9.4298	4.5639	-5.9112	79	C	18.5215	0.8444	-17.5700
16	C	-6.4807	-1.6273	7.0236	48	C	9.3257	3.7905	-7.0480	80	C	19.1898	1.9671	-16.8215
17	O	-8.6801	0.1415	4.6621	49	S	7.7999	2.9255	-7.0812	81	H	-15.0143	-5.0650	9.3800
18	O	-4.1209	-1.8593	7.1003	50	C	7.2912	3.6255	-5.5579	82	H	-12.9233	-6.2612	10.4278
19	C	-1.6462	0.5380	4.3893	51	C	8.2784	4.4570	-5.0811	83	H	-11.9263	-0.7344	8.4962
20	C	-1.9152	0.1254	3.1043	52	C	10.5839	5.4714	-5.5844	84	H	-6.2858	0.5411	3.8579
21	S	-3.5521	-0.4950	3.0196	53	C	10.6690	3.6864	-10.5849	85	H	-6.5117	-2.2160	7.9326
22	C	-3.8255	-0.1989	4.7263	54	C	12.0395	3.3904	-10.3868	86	H	-0.6895	0.9592	4.6729
23	C	-2.7137	0.3641	5.3148	55	C	12.4676	3.1957	-9.0703	87	H	0.3002	-0.6312	-0.9949
24	C	0.0588	-0.1131	-0.0749	56	C	9.8129	3.8098	-9.4949	88	H	2.6990	2.8866	1.2901
25	C	0.7465	1.0002	0.3487	57	C	10.2616	3.6397	-8.1726	89	H	-10.4424	-5.6817	10.9853
26	S	0.1027	1.5495	1.8797	58	C	11.6122	3.3107	-7.9781	90	H	-9.8613	-5.9077	9.3368
27	C	-1.0554	0.2284	1.9412	59	O	10.2709	3.8578	-11.8765	91	H	-8.9059	1.3031	7.3096
28	C	-0.9599	-0.5608	0.8083	60	O	12.1333	3.1023	-6.7178	92	H	-2.1788	-0.0121	7.3704
29	C	3.6945	3.1015	-0.6609	61	C	14.9577	3.4312	-12.7546	93	H	-1.9865	1.6709	6.8529
30	C	3.5446	2.5763	-1.9333	62	C	14.2320	2.6220	-13.5972	94	H	-1.2755	-2.4300	-0.1943
31	S	2.1992	1.4448	-1.9857	63	S	12.6549	2.3136	-12.9104	95	H	-1.9894	-2.3632	1.4209
32	C	1.8402	1.6922	-0.2916	64	C	13.0042	3.2833	-11.4925	96	H	4.4050	4.6417	0.6504

continues

### A3<sub>1</sub> geometry continuation

97	H	5.6899	3.6302	-0.0076	111	H	15.4786	5.5165	-11.0571	125	H	-10.4133	1.2546	6.4112
98	H	-10.2305	-0.2338	3.4096	112	H	12.3750	1.7751	-5.2021	126	H	-3.5952	1.0068	7.1753
99	H	-9.7884	-1.6219	4.4364	113	H	10.8197	1.6109	-6.0572	127	H	-2.7590	-1.5184	0.0796
100	H	-2.7032	-3.3095	7.1027	114	H	8.8313	4.2280	-13.2286	128	H	4.9216	4.8456	-1.0270
101	H	-4.2807	-3.8414	6.4630	115	H	8.2456	3.3578	-11.7879	129	H	-8.7606	-1.1741	3.0421
102	H	2.7837	2.5323	-4.6818	116	H	14.4306	0.9992	-18.0286	130	H	-3.2107	-2.8077	5.4696
103	H	5.0045	3.7498	-7.4682	117	H	12.1779	2.9638	-15.7141	131	H	3.3853	3.1675	-7.0628
104	H	4.6829	2.0188	-7.3858	118	H	12.3093	2.2221	-17.3144	132	H	11.0848	5.8200	-6.4888
105	H	8.1661	5.0172	-4.1610	119	H	20.2787	0.1496	-18.7206	133	H	14.1590	5.2138	-9.9204
106	H	10.2373	6.3437	-5.0248	120	H	18.7346	-1.6552	-19.8434	134	H	12.3276	1.0248	-6.8193
107	H	13.4971	2.9233	-8.8761	121	H	19.5941	1.6288	-15.8614	135	H	8.6085	5.1068	-11.6955
108	H	8.7773	4.0794	-9.6477	122	H	20.0240	2.3667	-17.4031	136	H	11.8688	1.2412	-15.9173
109	H	15.9533	3.7796	-13.0001	123	H	-9.6138	-4.3629	10.1494	137	H	18.4980	2.7853	-16.6152
110	H	15.6028	4.1998	-9.8946	124	H	-10.4464	1.4094	8.1751	138	H	11.3366	4.9542	-4.9837

### 6) A3<sub>2</sub>



1	C	-19.8675	4.7285	-1.3550	24	C	-4.5908	0.7426	-0.4915	47	C	6.3853	-4.0687	-0.1871
2	C	-19.3853	4.2606	-0.1486	25	C	-4.3489	-0.6113	-0.4886	48	C	7.0770	-2.9087	0.0907
3	S	-20.3043	4.9246	1.1930	26	S	-5.8589	-1.4852	-0.6139	49	S	5.9799	-1.6172	0.5445
4	C	-21.3360	5.8021	0.1189	27	C	-6.7876	0.0037	-0.7184	50	C	4.5785	-2.6549	0.3748
5	C	-20.9809	5.6077	-1.1825	28	C	-5.9580	1.1071	-0.6187	51	C	4.9802	-3.9084	-0.0262
6	C	-17.0062	1.6629	1.1857	29	C	-1.4471	-2.9998	-0.5019	52	C	7.0139	-5.3831	-0.5606
7	C	-16.0825	2.1325	0.2771	30	C	-0.6805	-1.9618	0.0000	53	C	10.5127	-1.8191	1.2448
8	S	-16.7489	3.4449	-0.6758	31	S	-1.6508	-0.5079	0.1944	54	C	11.3328	-2.1623	0.1426
9	C	-18.2916	3.3471	0.1451	32	C	-3.0888	-1.3105	-0.3956	55	C	10.7021	-2.7165	-0.9754
10	C	-18.2455	2.3614	1.1007	33	C	-2.7970	-2.6152	-0.7189	56	C	9.1442	-2.0678	1.2058
11	C	-12.4747	1.0701	0.7450	34	C	-19.3358	4.3578	-2.7140	57	C	8.5251	-2.6520	0.0859
12	C	-12.0841	0.7136	-0.5534	35	C	-16.7872	0.5121	2.1291	58	C	9.3322	-2.9594	-1.0206
13	C	-13.0293	0.8882	-1.5839	36	C	-11.2811	-1.9839	-2.0514	59	O	11.1459	-1.2671	2.3174
14	C	-13.7487	1.5491	1.0292	37	C	-6.4014	2.5452	-0.6705	60	O	8.8059	-3.5124	-2.1698
15	C	-14.7108	1.6721	0.0069	38	C	-0.9568	-4.3949	-0.7863	61	C	15.0698	-2.2623	-0.2409
16	C	-14.3101	1.3460	-1.2964	39	C	-14.0167	3.2478	2.6566	62	C	15.1107	-0.9695	0.2278
17	O	-14.0484	1.8519	2.3392	40	C	-11.9720	1.5592	-3.5929	63	S	13.4947	-0.4283	0.6154
18	O	-12.7347	0.5712	-2.8921	41	C	2.7088	-1.2458	1.4586	64	C	12.7898	-1.9592	0.1338
19	C	-8.9301	-1.1077	-1.5013	42	C	3.2243	-2.1733	0.5698	65	C	13.7689	-2.8327	-0.3009
20	C	-8.2238	-0.0961	-0.8914	43	S	1.9521	-2.8447	-0.4360	66	C	13.5444	-4.2553	-0.7435
21	S	-9.3412	1.0819	-0.2316	44	C	0.7165	-1.9082	0.3781	67	C	8.2012	-2.5716	-3.0634
22	C	-10.7336	0.1872	-0.8113	45	C	1.3010	-1.1101	1.3366	68	C	10.3805	-0.8966	3.4553
23	C	-10.3456	-0.9640	-1.4622	46	C	3.5027	-0.4811	2.4845	69	C	17.8601	1.4343	1.0759

continues



## A<sub>3</sub><sub>2</sub> geometry continuation

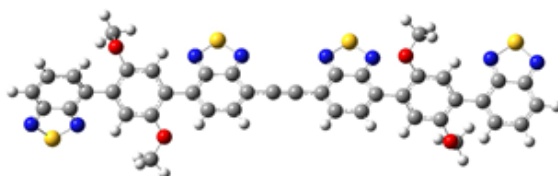
70	C	18.5463	0.9319	-0.0077	115	H	9.6239	-0.1456	3.2035	160	C	33.3625	11.1745	-3.4098
71	S	17.5665	-0.2768	-0.8113	116	H	18.2848	2.1853	1.7304	161	C	39.0197	10.7108	-1.2299
72	C	16.2719	-0.1099	0.3620	117	H	15.1573	0.4120	2.8648	162	C	39.3372	11.5090	-2.3039
73	C	16.5806	0.8608	1.2989	118	H	16.3255	1.6782	3.2655	163	S	37.9194	11.7612	-3.2968
74	C	15.7132	1.2610	2.4630	119	H	22.8511	1.0423	-1.9379	164	C	36.9094	10.8196	-2.2088
75	C	21.9682	1.4375	-1.4505	120	H	20.2078	-0.9576	-2.5030	165	C	37.6578	10.3121	-1.1610
76	C	21.8886	2.7372	-1.0070	121	H	21.7574	-1.2185	-1.7048	166	C	42.2446	13.4757	-3.6472
77	S	20.3354	3.0129	-0.2506	122	H	-18.8880	3.3630	-2.7163	167	C	43.0592	12.6684	-2.8717
78	C	19.8418	1.3448	-0.5054	123	H	-17.7179	-0.0410	2.2783	168	S	42.1028	11.4964	-1.9746
79	C	20.8251	0.6396	-1.1788	124	H	-16.4363	0.8600	3.1044	169	C	40.6081	12.0970	-2.6567
80	C	20.7528	-0.8142	-1.5641	125	H	-12.2518	-1.9685	-1.5543	170	C	40.8709	13.1409	-3.5129
81	H	-22.1407	6.4036	0.5126	126	H	-6.7576	2.8941	0.3044	171	C	24.2584	7.1480	-0.0876
82	H	-21.5042	6.0642	-2.0135	127	H	-0.2324	-4.7302	-0.0417	172	C	28.2369	6.0531	-5.4340
83	H	-19.1030	2.1132	1.7141	128	H	-13.0206	3.6649	2.4720	173	C	32.3598	12.0078	-4.1599
84	H	-11.7830	0.9494	1.5702	129	H	-10.9932	1.7106	-3.1280	174	C	37.1285	9.4626	-0.0360
85	H	-15.0163	1.4229	-2.1144	130	H	2.8563	-0.1680	3.3072	175	C	42.7137	14.5820	-4.5548
86	H	-8.4410	-1.9481	-1.9784	131	H	8.0222	-5.4724	-0.1535	176	C	30.8521	4.7314	-2.8192
87	H	-3.7955	1.4759	-0.4383	132	H	12.5939	-4.6481	-0.3818	177	C	31.0059	11.1360	-0.5808
88	H	-3.5398	-3.2961	-1.1160	133	H	8.9307	-1.8233	-3.3927	178	C	46.6784	11.8485	-2.2737
89	H	-20.1411	4.3691	-3.4526	134	H	9.8940	-1.7658	3.9113	179	C	46.9562	13.1892	-2.4753
90	H	-18.5710	5.0638	-3.0548	135	H	14.9821	2.0246	2.1773	180	S	45.4841	14.0877	-2.8006
91	H	-16.0347	-0.1795	1.7481	136	H	20.2512	-1.4122	-0.8009	181	C	44.4986	12.6430	-2.7123
92	H	-11.4619	-1.7914	-3.1122	137	H	7.0989	-5.4874	-1.6454	182	C	45.2949	11.5605	-2.4104
93	H	-10.8608	-2.9879	-1.9527	138	C	24.0347	5.8115	-0.7445	183	C	47.6970	10.7770	-1.9874
94	H	-5.5681	3.1876	-0.9628	139	C	24.8243	5.2602	-1.7379	184	C	49.8530	15.5417	-2.9584
95	H	-7.2117	2.6955	-1.3866	140	S	24.1987	3.6941	-2.2352	185	C	50.5113	14.8385	-1.9719
96	H	-1.7933	-5.0968	-0.7842	141	C	22.8682	3.7937	-1.1036	186	S	49.5202	13.5211	-1.3723
97	H	-0.4743	-4.4632	-1.7670	142	C	22.9409	4.9731	-0.3993	187	C	48.2141	13.9118	-2.4727
98	H	-14.2502	3.3256	3.7180	143	C	27.6655	6.1316	-4.0448	188	C	48.5599	15.0100	-3.2259
99	H	-14.7603	3.8049	2.0789	144	C	28.2366	6.8084	-2.9880	189	C	50.4270	16.7023	-3.7238
100	H	-11.8369	1.1804	-4.6057	145	S	27.2253	6.7121	-1.5591	190	C	54.0463	14.0853	-0.8491
101	H	-12.5118	2.5120	-3.6300	146	C	26.0135	5.7642	-2.3973	191	C	54.5012	15.3460	-0.3924
102	H	0.7208	-0.4560	1.9756	147	C	26.4160	5.5465	-3.6949	192	C	53.5941	16.4087	-0.4402
103	H	4.3134	-1.0826	2.9002	148	C	31.8770	7.8086	-3.3155	193	C	52.7571	13.9449	-1.3536
104	H	3.9506	0.4224	2.0577	149	C	31.8776	9.1355	-2.8624	194	C	51.8623	15.0281	-1.4222
105	H	4.2783	-4.7208	-0.1693	150	C	30.6549	9.6607	-2.3984	195	C	52.3012	16.2700	-0.9372
106	H	6.4147	-6.2145	-0.1812	151	C	30.7211	7.0365	-3.3429	196	O	54.9422	13.0611	-0.7806
107	H	11.2838	-2.9521	-1.8573	152	C	29.4880	7.5801	-2.9303	197	O	51.4832	17.3810	-0.9440
108	H	8.5288	-1.8451	2.0660	153	C	29.4948	8.8963	-2.4468	198	C	57.9271	16.5472	0.5798
109	H	15.9646	-2.8116	-0.5064	154	O	30.8138	5.7495	-3.8253	199	C	58.0148	15.4742	1.4355
110	H	13.5469	-4.3441	-1.8354	155	O	30.5588	10.9521	-1.9281	200	S	56.5650	14.5051	1.3218
111	H	14.3438	-4.8988	-0.3664	156	C	34.7060	11.5949	-3.1996	201	C	55.8626	15.5694	0.1190
112	H	7.8560	-3.1436	-3.9245	157	C	35.4978	10.6996	-2.5173	202	C	56.7192	16.6153	-0.1677
113	H	7.3489	-2.0694	-2.5955	158	S	34.5597	9.2732	-2.1211	203	C	56.4753	17.6975	-1.1872
114	H	11.0910	-0.4709	4.1617	159	C	33.1170	9.9295	-2.8717	204	C	50.5581	17.4495	0.1463

continues

### A<sub>3</sub><sub>2</sub> geometry continuation

205	C	54.5481	11.7688	-1.2192	229	H	32.8545	12.5807	-4.9482	253	H	58.7857	12.6117	1.2667
206	C	60.7078	14.0954	3.6527	230	H	37.7912	9.5256	0.8295	254	H	59.9464	11.8586	2.3685
207	C	61.0440	15.3965	3.9427	231	H	36.1315	9.7782	0.2777	255	H	64.5674	17.8166	5.9642
208	S	59.9504	16.4848	3.1182	232	H	41.9658	14.7811	-5.3251	256	H	64.1848	15.8887	7.7077
209	C	59.0920	15.1570	2.3561	233	H	42.8754	15.5157	-4.0060	257	H	62.3115	18.7851	3.7737
210	C	59.6115	13.9407	2.7605	234	H	30.9447	3.7828	-3.3472	258	H	63.9910	18.3322	3.4902
211	C	59.1362	12.5880	2.3000	235	H	29.9357	4.7271	-2.2215	259	H	24.6607	7.8817	-0.7884
212	C	63.8166	17.0422	5.8674	236	H	30.8533	12.1896	-0.3484	260	H	27.4343	6.0260	-6.1752
213	C	63.6431	16.0533	6.7891	237	H	30.4177	10.5223	0.1105	261	H	28.8502	5.1570	-5.5606
214	S	62.3688	14.9790	6.3304	238	H	44.8967	10.5573	-2.3223	262	H	31.5897	11.3870	-4.6195
215	C	62.0794	15.8720	4.8452	239	H	48.6362	10.9603	-2.5128	263	H	37.0627	8.4076	-0.3220
216	C	62.9318	16.9551	4.7489	240	H	47.9264	10.7128	-0.9186	264	H	43.6519	14.3286	-5.0521
217	C	62.9801	17.9340	3.6057	241	H	47.9085	15.4125	-3.9918	265	H	31.7183	4.8678	-2.1622
218	H	22.2208	5.2396	0.3646	242	H	50.0380	16.7163	-4.7450	266	H	32.0670	10.8907	-0.4760
219	H	25.8043	5.0043	-4.4055	243	H	53.8853	17.3795	-0.0600	267	H	47.3184	9.8013	-2.2994
220	H	32.7928	7.3630	-3.6852	244	H	52.4284	12.9910	-1.7415	268	H	51.5156	16.6486	-3.7714
221	H	28.5702	9.3573	-2.1207	245	H	58.7325	17.2613	0.4609	269	H	55.7132	17.4091	-1.9115
222	H	35.0803	12.5503	-3.5462	246	H	56.1491	18.6308	-0.7153	270	H	51.0875	17.4668	1.1054
223	H	39.7451	10.4374	-0.4734	247	H	57.3969	17.9175	-1.7325	271	H	54.2948	11.7673	-2.2850
224	H	40.0878	13.6723	-4.0397	248	H	50.0047	18.3801	0.0219	272	H	58.3103	12.2191	2.9172
225	H	23.3175	7.5373	0.3071	249	H	49.8603	16.6067	0.1296	273	H	62.6888	17.4703	2.6620
226	H	24.9599	7.0753	0.7501	250	H	55.4113	11.1264	-1.0541	274	H	50.1764	17.6537	-3.2474
227	H	28.8762	6.9096	-5.6520	251	H	53.6977	11.3904	-0.6416					
228	H	31.8497	12.7099	-3.4951	252	H	61.2639	13.2544	4.0484					

### 7) B<sub>1</sub>



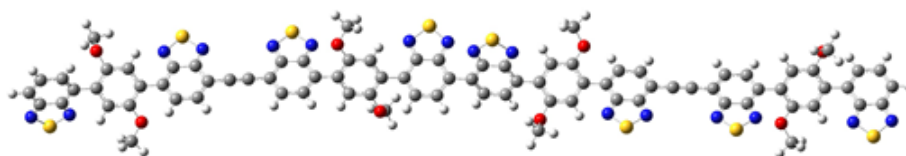
1	C	-10.7552	-0.0933	-0.7492	15	C	-8.6174	1.1575	-0.3876	29	C	-9.1483	-3.3010	0.0946
2	C	-11.6073	0.6940	0.1055	16	O	-9.0501	-2.4377	-1.0422	30	C	-7.3491	3.5726	0.2772
3	C	-13.0529	0.6438	-0.0444	17	O	-6.5824	2.4187	-0.0456	31	C	4.9213	0.5302	-0.2789
4	C	-13.6493	-0.1732	-1.0417	18	C	-2.0248	0.1790	-0.2859	32	C	4.2619	-0.5699	0.3627
5	C	-12.8152	-0.9061	-1.8382	19	C	-2.7569	-0.8936	0.3297	33	C	2.8142	-0.6637	0.3787
6	C	-11.3973	-0.8681	-1.6923	20	C	-4.2094	-0.9262	0.2838	34	C	2.0069	0.3510	-0.2456
7	N	-11.2160	1.5041	1.0946	21	C	-4.9552	0.1179	-0.3694	35	C	2.6882	1.4030	-0.8313
8	S	-12.5744	2.1372	1.7609	22	C	-4.1990	1.1285	-0.9316	36	C	4.1044	1.4860	-0.8418
9	N	-13.7098	1.4140	0.8276	23	C	-2.7845	1.1600	-0.8984	37	N	4.8593	-1.5685	1.0170
10	C	-7.0989	-1.1202	-0.6808	24	N	-2.2163	-1.9195	0.9838	38	S	3.6674	-2.5413	1.5790
11	C	-6.4318	0.0845	-0.4444	25	S	-3.4580	-2.8506	1.5036	39	N	2.3537	-1.7326	1.0257
12	C	-7.2323	1.2436	-0.2935	26	N	-4.7212	-1.9867	0.9167	40	C	8.6065	-0.1699	-0.8561
13	C	-8.4826	-1.2061	-0.7779	27	C	-0.6138	0.2209	-0.2596	41	C	9.2205	0.9686	-0.3078
14	C	-9.2785	-0.0574	-0.6308	28	C	0.5965	0.2727	-0.2476	42	C	8.3896	1.9581	0.2439

continues

## B<sub>1</sub> geometry continuation

43	C	7.2239	-0.3297	-0.8622	57	C	7.3610	-2.4936	-1.8753	71	H	4.5623	2.3338	-1.3387
44	C	6.3964	0.6612	-0.2936	58	C	9.2145	3.0345	2.1817	72	H	9.2361	-0.9306	-1.2901
45	C	7.0071	1.7935	0.2420	59	H	-14.7265	-0.1956	-1.1433	73	H	6.3997	2.5709	0.6907
46	O	8.9071	3.1194	0.7874	60	H	-13.2313	-1.5396	-2.6134	74	H	10.6792	3.1723	-0.8720
47	O	6.5877	-1.3839	-1.4385	61	H	-10.7996	-1.4804	-2.3524	75	H	13.1073	3.4482	-1.0183
48	C	13.5817	1.4398	-0.5146	62	H	-6.5274	-2.0291	-0.8040	76	H	7.9681	-2.8998	-1.0602
49	C	13.0205	0.1790	-0.1777	63	H	-9.2165	2.0445	-0.2599	77	H	8.0096	-2.2254	-2.7169
50	C	11.5789	0.0069	-0.1029	64	H	-4.7089	1.9413	-1.4285	78	H	9.9810	2.2757	2.3728
51	C	10.6956	1.1149	-0.3598	65	H	-2.2744	1.9868	-1.3778	79	H	8.3192	2.7967	2.7667
52	C	11.3029	2.3113	-0.6767	66	H	-9.8161	-2.8761	0.8522	80	H	14.6567	1.5509	-0.5709
53	C	12.7179	2.4714	-0.7547	67	H	-8.1647	-3.4789	0.5417	81	H	-9.5600	-4.2432	-0.2667
54	N	13.7081	-0.9326	0.0998	68	H	-7.9988	3.3909	1.1392	82	H	-6.6243	4.3468	0.5237
55	S	12.6024	-2.0954	0.4309	69	H	-7.9561	3.9036	-0.5727	83	H	6.6422	-3.2427	-2.2028
56	N	11.2200	-1.2361	0.2339	70	H	2.1173	2.1897	-1.3093	84	H	9.5912	4.0138	2.4768

## 8) B<sub>2</sub>

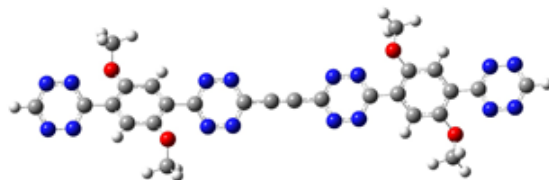


1	C	-10.8100	0.2308	-0.6023	25	S	-3.6259	-1.8804	2.5372	49	C	12.9603	-0.4172	-0.0495
2	C	-11.6162	1.3084	-0.0872	26	N	-4.8538	-1.2249	1.6716	50	C	11.5138	-0.4653	0.0931
3	C	-13.0641	1.2759	-0.2195	27	C	-0.6608	0.2276	-0.1832	51	C	10.6733	0.5023	-0.5613
4	C	-13.7076	0.1879	-0.8676	28	C	0.5506	0.2255	-0.1824	52	C	11.3312	1.4615	-1.3008
5	C	-12.9162	-0.8174	-1.3477	29	C	-9.3438	-2.5432	1.3322	53	C	12.7454	1.4994	-1.4464
6	C	-11.4966	-0.7965	-1.2149	30	C	-7.2282	3.8596	-0.9153	54	N	13.5965	-1.3453	0.6670
7	N	-11.1781	2.3965	0.5543	31	C	4.8820	0.2566	-0.2824	55	S	12.4468	-2.2188	1.4356
8	S	-12.4991	3.2870	0.9443	32	C	4.1824	-0.4833	0.7274	56	N	11.1031	-1.4463	0.9026
9	N	-13.6760	2.3344	0.3192	33	C	2.7321	-0.4987	0.7690	57	C	7.1672	-3.2556	-0.5850
10	C	-7.2044	-0.8749	-0.1496	34	C	1.9630	0.2353	-0.2009	58	C	9.3012	3.3209	1.0472
11	C	-6.4804	0.3031	-0.3501	35	C	2.6832	0.9519	-1.1400	59	H	-14.7856	0.1812	-0.9622
12	C	-7.2250	1.4766	-0.6246	36	C	4.1014	0.9606	-1.1729	60	H	-13.3688	-1.6639	-1.8516
13	C	-8.5916	-0.9249	-0.2199	37	N	4.7427	-1.1811	1.7180	61	H	-10.9345	-1.6298	-1.6116
14	C	-9.3321	0.2374	-0.4940	38	S	3.5159	-1.8101	2.6022	62	H	-6.6766	-1.7941	0.0607
15	C	-8.6134	1.4275	-0.6918	39	N	2.2326	-1.2166	1.7731	63	H	-9.1698	2.3293	-0.8902
16	O	-9.2180	-2.1424	-0.0356	40	C	8.5252	-0.7776	-0.5301	64	H	-4.6838	1.6051	-1.9187
17	O	-6.5189	2.6316	-0.8041	41	C	9.1956	0.4552	-0.4596	65	H	-2.2494	1.5528	-1.8698
18	C	-2.0724	0.2437	-0.2032	42	C	8.4156	1.6171	-0.3336	66	H	-9.9834	-1.8475	1.8866
19	C	-2.8470	-0.5041	0.7488	43	C	7.1372	-0.8649	-0.4793	67	H	-8.3649	-2.5976	1.8196
20	C	-4.2998	-0.4840	0.7065	44	C	6.3611	0.3047	-0.3386	68	H	-7.8770	4.0247	-0.0494
21	C	-5.0031	0.2922	-0.2813	45	C	7.0275	1.5271	-0.2773	69	H	-7.8276	3.8969	-1.8316
22	C	-4.2069	1.0000	-1.1612	46	O	8.9909	2.8732	-0.2753	70	H	2.1419	1.5209	-1.8861
23	C	-2.7922	0.9757	-1.1310	47	O	6.4483	-2.0297	-0.6086	71	H	4.5902	1.5320	-1.9537
24	N	-2.3478	-1.2537	1.7294	48	C	13.5869	0.5835	-0.8607	72	H	9.1154	-1.6740	-0.6373

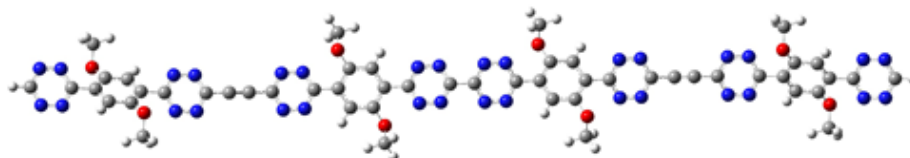
continues

## B<sub>2</sub> geometry continuation

73	H	6.4604	2.4437	-0.1645	105	C	24.6011	0.6661	-0.7146	137	N	42.1689	4.1638	-2.9833
74	H	10.7479	2.2185	-1.8060	106	C	26.0094	0.7990	-0.7550	138	S	40.9520	4.8435	-3.8442
75	H	13.1714	2.2706	-2.0784	107	N	26.2935	2.6204	-3.9094	139	N	39.6720	4.0399	-3.2086
76	H	7.7679	-3.3460	0.3255	108	S	24.9750	3.0197	-4.7932	140	C	35.5936	5.7022	-1.9733
77	H	7.8146	-3.3592	-1.4630	109	N	23.7975	2.3999	-3.8359	141	C	38.2775	-0.8400	-2.6492
78	H	10.0315	2.6609	1.5276	110	C	28.0805	1.5711	-1.8117	142	H	15.2536	2.6455	-0.3555
79	H	8.3988	3.3696	1.6665	111	C	29.2877	1.6710	-1.8199	143	H	17.6693	2.7951	-0.6445
80	H	-9.8023	-3.5319	1.3243	112	C	19.2397	3.3990	-3.6779	144	H	21.9248	3.0452	-2.3206
81	H	-6.4660	4.6362	-0.9532	113	C	21.8187	-2.4279	-0.5160	145	H	19.7618	-1.0784	-0.7592
82	H	6.4123	-4.0398	-0.6030	114	C	33.6066	2.0084	-1.7452	146	H	24.1690	0.1406	0.1247
83	H	9.7254	4.3198	0.9454	115	C	32.8540	2.5352	-2.8465	147	H	26.5916	0.3800	0.0568
84	C	17.9626	0.8146	-1.3459	116	C	31.4076	2.4258	-2.8802	148	H	18.6761	2.5821	-4.1420
85	C	17.2483	-0.3900	-1.6811	117	C	30.6961	1.7791	-1.8094	149	H	20.2232	3.4720	-4.1534
86	C	15.8033	-0.4678	-1.5335	118	C	31.4676	1.2666	-0.7817	150	H	21.1914	-2.7718	-1.3444
87	C	15.0530	0.6444	-1.0317	119	C	32.8816	1.3788	-0.7574	151	H	21.2177	-2.3755	0.3984
88	C	15.7748	1.7792	-0.7474	120	N	33.3604	3.1262	-3.9311	152	H	30.9709	0.7689	0.0423
89	C	17.1859	1.8633	-0.9010	121	S	32.0908	3.5186	-4.8885	153	H	33.4115	0.9678	0.0944
90	N	17.7794	-1.5091	-2.1833	122	N	30.8561	2.9481	-3.9739	154	H	37.6654	4.3101	-1.7079
91	S	16.5402	-2.5488	-2.4507	123	C	37.1515	3.3623	-1.6779	155	H	35.3600	-0.0362	-1.5566
92	N	15.2876	-1.6275	-1.9439	124	C	37.9210	2.1915	-1.5749	156	H	39.5988	0.7906	0.0142
93	C	21.4700	2.1279	-1.9750	125	C	37.2399	0.9636	-1.5246	157	H	42.0324	0.9364	0.2367
94	C	22.2846	1.0541	-1.6067	126	C	35.7610	3.3273	-1.7291	158	H	36.1876	5.7071	-2.8927
95	C	21.6341	-0.1220	-1.1581	127	C	35.0844	2.0901	-1.6930	159	H	36.2278	5.9862	-1.1259
96	C	20.0829	2.0764	-1.9069	128	C	35.8492	0.9305	-1.5821	160	H	38.9563	-0.1965	-3.2191
97	C	19.4355	0.9117	-1.4605	129	O	37.9163	-0.2363	-1.4038	161	H	37.3891	-1.0513	-3.2545
98	C	20.2460	-0.1747	-1.0923	130	O	34.9783	4.4383	-1.7639	162	H	43.3685	2.5153	-1.1500
99	O	19.3611	3.1982	-2.2664	131	C	42.2919	2.4456	-1.2356	163	H	18.7002	4.3364	-3.8120
100	O	22.4287	-1.1775	-0.8131	132	C	41.6038	3.2743	-2.1618	164	H	22.6401	-3.1267	-0.3662
101	C	26.6746	1.4447	-1.7823	133	C	40.1574	3.2007	-2.2879	165	H	34.7767	6.4161	-2.0632
102	C	25.8491	1.9827	-2.8285	134	C	39.3987	2.2792	-1.4822	166	H	38.7818	-1.7752	-2.4062
103	C	24.4023	1.8528	-2.7767	135	C	40.1260	1.5009	-0.6071					
104	C	23.7566	1.1734	-1.6836	136	C	41.5444	1.5829	-0.4840					

9) C<sub>1</sub>

1	N	12.2077	1.3671	0.4720	23	N	-2.6358	-1.2185	-0.7599	45	C	0.6034	0.0042	-0.6266
2	N	12.2170	-0.9755	0.8630	24	N	-2.6685	1.1540	-0.5093	46	C	-0.6021	-0.0040	-0.6262
3	C	12.8222	0.2051	0.7001	25	C	-2.0223	-0.0243	-0.6152	47	H	13.9010	0.2253	0.7959
4	N	10.9019	1.3324	0.3020	26	N	-3.9391	-1.2456	-0.6540	48	H	8.5391	2.0075	1.1339
5	C	10.2883	0.1385	0.3854	27	C	-4.5796	-0.0888	-0.3804	49	H	6.3271	-1.7817	-1.1314
6	N	10.9111	-1.0109	0.7157	28	N	-3.9718	1.1131	-0.3815	50	H	9.2824	-3.2516	0.5424
7	C	8.0548	1.1852	0.6233	29	C	-6.8101	0.9604	-0.6146	51	H	7.8118	-3.6041	-0.4242
8	C	6.6718	1.1951	0.4774	30	C	-8.1921	0.9693	-0.4663	52	H	5.5819	3.4855	-0.5245
9	C	6.0373	0.1141	-0.1658	31	C	-8.8256	-0.1127	0.1747	53	H	7.0562	3.8297	0.4389
10	C	8.8275	0.1125	0.1684	32	C	-6.0357	-0.1141	-0.1615	54	H	-6.3262	1.7822	-1.1260
11	C	8.1935	-0.9692	-0.4726	33	C	-6.6697	-1.1955	0.4816	55	H	-8.5366	-2.0081	1.1391
12	C	6.8114	-0.9602	-0.6200	34	C	-8.0527	-1.1856	0.6285	56	H	-13.8987	-0.2257	0.8058
13	O	8.9461	-1.9548	-1.0480	35	O	-8.9451	1.9552	-1.0407	57	H	-7.0541	-3.8300	0.4421
14	O	5.9214	2.1788	1.0573	36	O	-5.9189	-2.1794	1.0606	58	H	-5.5805	-3.4854	-0.5221
15	N	2.6370	1.2188	-0.7612	37	N	-12.2147	0.9750	0.8722	59	H	-9.2802	3.2512	0.5506
16	N	2.6699	-1.1539	-0.5117	38	N	-12.2056	-1.3674	0.4800	60	H	-7.8104	3.6042	-0.4169
17	C	2.0236	0.0245	-0.6167	39	C	-12.8200	-0.2055	0.7092	61	H	9.4284	-3.9221	-1.1046
18	N	3.9404	1.2459	-0.6562	40	N	-10.9089	1.0105	0.7240	62	H	5.4420	4.1465	1.1266
19	C	4.5811	0.0888	-0.3837	41	C	-10.2862	-0.1387	0.3927	63	H	-5.4395	-4.1471	1.1285
20	N	3.9732	-1.1130	-0.3849	42	N	-10.9000	-1.3326	0.3092	64	H	-9.4275	3.9225	-1.0960
21	C	8.8501	-3.2612	-0.4611	43	C	-6.0154	-3.4889	0.4803					
22	C	6.0175	3.4886	0.4776	44	C	-8.8487	3.2613	-0.4533					

10) C<sub>2</sub>

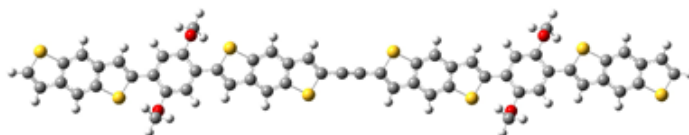
1	N	-10.7998	-1.0601	1.1474	13	O	-7.5287	1.4394	-1.5766	25	C	3.4153	-0.2083	-0.5521
2	N	-10.8330	1.2287	0.5098	14	O	-4.5438	-1.6370	1.9307	26	N	5.3237	0.9854	-0.8654
3	C	-11.4244	0.0844	0.8637	15	N	-1.2327	-1.4130	-0.0853	27	C	5.9768	-0.1090	-0.4204
4	N	-9.4944	-1.0877	0.9731	16	N	-1.2816	0.8578	-0.8222	28	N	5.3739	-1.2891	-0.1797
5	C	-8.8922	0.0357	0.5423	17	C	-0.6301	-0.2624	-0.4511	29	C	8.1895	-1.2127	-0.5213
6	N	-9.5259	1.2111	0.3584	18	N	-2.5364	-1.4009	0.0329	30	C	9.5764	-1.2149	-0.4296
7	C	-6.6635	-0.8539	1.1538	19	C	-3.1837	-0.2371	-0.1893	31	C	10.2440	-0.0349	-0.0440
8	C	-5.2812	-0.9297	1.0247	20	N	-2.5838	0.8663	-0.6773	32	C	7.4414	-0.0564	-0.2722
9	C	-4.6400	-0.1770	0.0200	21	C	-7.4554	2.8690	-1.4769	33	C	8.1095	1.1237	0.1137
10	C	-7.4315	-0.0236	0.3318	22	C	-4.6234	-3.0672	1.8420	34	C	9.4966	1.1212	0.2050
11	C	-6.7910	0.7297	-0.6720	23	N	4.0164	0.9426	-0.9199	35	O	10.2917	-2.3113	-0.8163
12	C	-5.4093	0.6547	-0.8022	24	N	4.0670	-1.3500	-0.2534	36	O	7.3960	2.2213	0.5007

continues

## C<sub>2</sub> geometry continuation

46	C	1.9951	-0.2306	-0.5233	79	N	25.9419	1.6174	-0.2535	103	N	39.5348	-0.9438	0.3582
47	H	-12.5030	0.0964	0.9620	80	C	26.5936	0.4757	-0.5521	104	C	38.9012	0.2316	0.5422
48	H	-7.1518	-1.4221	1.9345	81	N	24.6852	-0.7180	-0.8655	105	N	39.5033	1.3550	0.9730
49	H	-4.9216	1.2220	-1.5836	82	C	24.0321	0.3764	-0.4205	106	C	34.6324	3.3345	1.8420
50	H	-7.9180	3.2034	-0.5454	83	N	24.6350	1.5565	-0.1798	107	C	37.4643	-2.6016	-1.4771
51	H	-6.4195	3.2176	-1.5344	84	C	19.7777	3.7216	0.0501	108	C	28.0139	0.4980	-0.5234
52	H	-4.1641	-3.4108	0.9123	85	C	22.5554	-3.0943	-0.3692	109	C	29.2189	0.5132	-0.4937
53	H	-5.6606	-3.4109	1.9036	86	N	31.2416	1.6803	-0.0853	110	H	20.0021	-1.7561	0.5152
54	H	7.6792	-2.1145	-0.8325	87	N	31.2905	-0.5904	-0.8223	111	H	22.3297	2.3819	-0.8325
55	H	10.0068	2.0234	0.5153	88	C	30.6390	0.5298	-0.4512	112	H	19.2882	3.4968	1.0006
56	H	8.4875	3.6737	-0.5456	89	N	32.5453	1.6683	0.0328	113	H	20.8120	4.0363	0.2196
57	H	6.9579	3.1355	-1.3159	90	C	33.1927	0.5044	-0.1894	114	H	23.0510	-2.8681	-1.3161
58	H	10.7208	-3.2295	1.0005	91	N	32.5927	-0.5989	-0.6774	115	H	21.5214	-3.4063	-0.5458
59	H	9.1969	-3.7689	0.2195	92	C	35.4183	-0.3873	-0.8023	116	H	34.9305	-0.9546	-1.5838
60	H	-8.0163	3.2580	-2.3252	93	C	36.7999	-0.4623	-0.6721	117	H	37.1607	1.6894	1.9345
61	H	-4.0622	-3.4520	2.6919	94	C	37.4405	0.2910	0.3316	118	H	42.5119	0.1709	0.9619
62	H	6.9168	4.1575	0.1446	95	C	34.6489	0.4444	0.0199	119	H	35.6695	3.6782	1.9037
63	H	10.7729	-4.2473	-0.4625	96	C	35.2901	1.1971	1.0246	120	H	34.1730	3.6782	0.9123
64	N	16.3855	-0.9779	-0.0718	97	C	36.6724	1.1213	1.1537	121	H	37.9270	-2.9360	-0.5457
65	N	16.3421	1.2928	0.6312	98	O	37.5376	-1.1719	-1.5768	122	H	36.4284	-2.9501	-1.5346
66	C	15.7460	0.1500	0.2600	99	O	34.5528	1.9043	1.9306	123	H	19.2361	4.5147	-0.4623
76	O	19.7172	2.5787	-0.8162	100	N	40.8419	-0.9613	0.5097	124	H	23.0921	-3.8901	0.1444
77	O	22.6129	-1.9539	0.5005	101	N	40.8087	1.3274	1.1473	125	H	34.0711	3.7192	2.6919
78	N	25.9925	-0.6752	-0.9200	102	C	41.4333	0.1830	0.8635	126	H	38.0252	-2.9905	-2.3254

## 11) D<sub>1</sub>



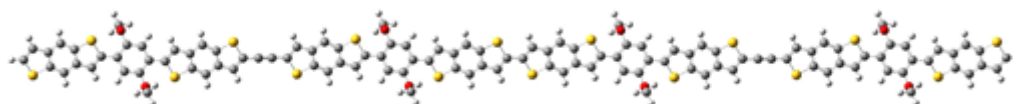
1	C	13.2224	2.9964	-1.5163	15	C	2.8670	-0.9922	-0.3409	29	C	11.1296	1.0991	-0.0845
2	C	10.6679	-3.0338	1.5786	16	C	2.0068	0.0046	0.0355	30	C	10.5091	-0.1535	0.0445
3	C	18.4971	1.4033	0.5640	17	S	2.8711	1.4447	0.6167	31	C	13.3591	0.1279	0.0215
4	C	19.6220	0.6228	0.2718	18	C	0.6070	-0.0059	0.0071	32	C	12.7387	-1.1245	0.1499
5	C	19.4482	-0.6852	-0.2679	19	C	5.6743	1.2050	0.5723	33	C	11.3596	-1.2719	0.1525
6	C	18.1948	-1.2240	-0.5161	20	C	6.7990	0.4202	0.2809	34	O	13.0373	2.5154	-0.1789
7	C	17.0705	-0.4435	-0.2171	21	C	6.6267	-0.8966	-0.2361	35	O	10.8294	-2.5404	0.2426
8	C	17.2424	0.8643	0.3198	22	C	5.3732	-1.4400	-0.4678	36	C	-0.6070	0.0066	-0.0087
9	C	21.0137	0.9511	0.4382	23	C	4.2466	-0.6549	-0.1829	37	C	-8.1819	-0.7497	-0.4359
10	C	21.8453	-0.0434	0.0490	24	C	4.4210	0.6631	0.3374	38	C	-9.0456	0.2433	-0.0656
11	S	21.0048	-1.4589	-0.5505	25	C	8.1819	0.7500	0.4352	39	S	-8.1759	1.6865	0.4896
12	C	15.6861	-0.7703	-0.3797	26	C	9.0456	-0.2431	0.0649	40	C	-5.3732	1.4406	0.4664
13	C	14.8230	0.2172	0.0030	27	S	8.1759	-1.6861	-0.4906	41	C	-4.2466	0.6556	0.1814
14	S	15.6930	1.6514	0.5818	28	C	12.5086	1.2465	-0.0875	42	C	-4.4210	-0.6626	-0.3386

continues

## D<sub>1</sub> geometry continuation

43	C	-5.6743	-1.2046	-0.5732	64	C	-10.5090	0.1537	-0.0448	85	H	-8.5165	-1.7007	-0.8292
44	C	-6.7990	-0.4198	-0.2819	65	C	-11.1295	-1.0990	0.0844	86	H	-5.2556	2.4441	0.8587
45	C	-6.6267	0.8970	0.2349	66	C	-12.5084	-1.2465	0.0878	87	H	-5.7916	-2.2068	-0.9688
46	C	-2.8670	0.9929	0.3392	67	O	-10.8296	2.5405	-0.2429	88	H	-2.5188	1.9440	0.7191
47	C	-2.0068	-0.0039	-0.0371	68	O	-13.0370	-2.5154	0.1794	89	H	-21.3606	-1.8975	-0.8325
48	S	-2.8711	-1.4442	-0.6180	69	C	-10.6685	3.0339	-1.5790	90	H	-22.9247	0.0483	-0.0688
49	C	-21.0137	-0.9519	-0.4366	70	C	-13.2221	-2.9961	1.5169	91	H	-18.0790	2.2196	0.9284
50	C	-21.8453	0.0425	-0.0472	71	H	13.9085	2.3520	-2.0748	92	H	-18.6128	-2.4014	-0.9711
51	S	-21.0049	1.4580	0.5522	72	H	10.2389	-4.0307	1.4878	93	H	-15.3515	1.7148	0.7885
52	C	-18.1949	1.2234	0.5173	73	H	9.9899	-2.3955	2.1539	94	H	-13.3397	2.0180	-0.2632
53	C	-17.0704	0.4430	0.2181	74	H	18.6129	2.4009	0.9722	95	H	-10.5296	-1.9932	0.1982
54	C	-17.2424	-0.8647	-0.3188	75	H	18.0789	-2.2202	-0.9271	96	H	-10.2391	4.0307	-1.4883
55	C	-18.4970	-1.4039	-0.5628	76	H	21.3607	1.8967	0.8342	97	H	-9.9909	2.3955	-2.1546
56	C	-19.6220	-0.6235	-0.2704	77	H	22.9247	-0.0494	0.0708	98	H	-13.6518	-3.9929	1.4281
57	C	-19.4482	0.6845	0.2694	78	H	15.3515	-1.7151	-0.7877	99	H	-13.9082	-2.3515	2.0753
58	C	-15.6861	0.7700	0.3805	79	H	2.5188	-1.9432	-0.7210	100	H	13.6520	3.9932	-1.4272
59	C	-14.8230	-0.2174	-0.0024	80	H	5.7917	2.2071	0.9681	101	H	12.2643	3.0546	-2.0434
60	S	-15.6929	-1.6517	-0.5812	81	H	5.2556	-2.4434	-0.8604	102	H	11.6345	-3.0947	2.0893
61	C	-11.3597	1.2720	-0.1527	82	H	8.5165	1.7008	0.8287	103	H	-11.6352	3.0951	-2.0893
62	C	-12.7388	1.1244	-0.1498	83	H	10.5298	1.9933	-0.1983	104	H	-12.2641	-3.0543	2.0440
63	C	-13.3591	-0.1280	-0.0212	84	H	13.3395	-2.0181	0.2634					

## 12) D<sub>2</sub>



1	C	13.0162	3.3686	-1.7167	19	C	5.6290	1.1765	0.5031	37	C	-8.2344	-0.8619	-0.1388
2	C	10.7285	-3.0362	0.7780	20	C	6.7503	0.4553	0.0693	38	C	-9.0887	0.0643	0.3918
3	C	18.4266	1.6735	-0.1153	21	C	6.5737	-0.7943	-0.5926	39	S	-8.2066	1.4348	1.0926
4	C	19.5495	0.9526	-0.5423	22	C	5.3189	-1.3324	-0.8303	40	C	-5.4058	1.2297	0.9216
5	C	19.3714	-0.2990	-1.2020	23	C	4.1954	-0.6100	-0.4032	41	C	-4.2867	0.5027	0.4906
6	C	18.1196	-0.8402	-1.4396	24	C	4.3744	0.6405	0.2623	42	C	-4.4734	-0.7398	-0.1874
7	C	16.9963	-0.1198	-1.0063	25	C	8.1337	0.7939	0.1977	43	C	-5.7316	-1.2633	-0.4375
8	C	17.1715	1.1314	-0.3492	26	C	8.9938	-0.1298	-0.3278	44	C	-6.8486	-0.5371	-0.0007
9	C	20.9325	1.2967	-0.4140	27	S	8.1210	-1.5153	-1.0103	45	C	-6.6640	0.7044	0.6743
10	C	21.7918	0.3744	-0.9411	28	C	12.4196	1.4436	-0.4701	46	C	-2.9043	0.8354	0.6320
11	S	20.9220	-1.0047	-1.6422	29	C	11.0452	1.2662	-0.4188	47	C	-2.0536	-0.0930	0.0938
12	C	15.6134	-0.4611	-1.1327	30	C	10.4527	-0.0064	-0.4062	48	S	-2.9311	-1.4582	-0.6307
13	C	14.7520	0.4632	-0.6098	31	C	13.2932	0.3392	-0.5314	49	C	-21.0538	-1.2128	0.3495
14	S	15.6240	1.8513	0.0680	32	C	12.7006	-0.9334	-0.5188	50	C	-21.8749	-0.2882	0.8999
15	C	2.8150	-0.9540	-0.5385	33	C	11.3262	-1.1108	-0.4678	51	S	-21.0193	1.0454	1.6474
16	C	1.9588	-0.0262	-0.0080	34	O	12.9228	2.7256	-0.4390	52	C	-18.2117	0.8499	1.4697
17	S	2.8280	1.3519	0.7021	35	O	10.8225	-2.3926	-0.4995	53	C	-17.0957	0.1289	1.0252
18	C	0.5594	-0.0595	0.0238	36	C	-0.6541	-0.0655	0.0627	54	C	-17.2814	-1.0985	0.3273

continues

## D<sub>2</sub> geometry continuation

55	C	-18.5417	-1.6152	0.0643	100	H	12.0267	3.4657	-2.1753	145	C	40.6531	0.1536	-2.1754
56	C	-19.6585	-0.8932	0.5021	101	H	11.7178	-3.1335	1.2370	146	C	39.3992	-0.3860	-2.4120
57	C	-19.4708	0.3340	1.2028	102	H	-11.7830	3.1258	-1.1310	147	C	38.2768	0.3369	-1.9839
58	C	-15.7080	0.4478	1.1737	103	H	-12.1962	-3.5193	2.1817	148	C	38.4517	1.5919	-1.3317
59	C	-14.8552	-0.4703	0.6292	104	C	58.1880	4.2396	-3.6519	149	C	42.2100	1.7566	-1.3872
60	S	-15.7392	-1.8259	-0.0986	105	C	55.8327	-2.1652	-1.2232	150	C	43.0677	0.8261	-1.9105
61	C	-11.4111	1.0674	0.5349	106	C	63.5623	2.4834	-2.0013	151	S	42.2005	-0.5588	-2.6097
62	C	-12.7879	0.9042	0.5746	107	C	64.6816	1.7623	-2.4340	152	C	24.0946	-0.5134	-1.4962
63	C	-13.3940	-0.3617	0.5630	108	C	64.4981	0.5287	-3.1246	153	C	23.2347	0.4137	-0.9788
64	C	-10.5493	-0.0451	0.4604	109	C	63.2409	0.0059	-3.3865	154	S	24.1035	1.8006	-0.2920
65	C	-11.1556	-1.3113	0.4496	110	C	62.1224	0.7261	-2.9471	155	C	26.9061	1.6347	-0.4903
66	C	-12.5322	-1.4745	0.4897	111	C	62.3039	1.9598	-2.2592	156	C	28.0299	0.9108	-0.9162
67	O	-10.8936	2.3430	0.5901	112	C	66.0758	2.0884	-2.2849	157	C	27.8556	-0.3467	-1.5614
68	O	-13.0481	-2.7508	0.4357	113	C	66.9000	1.1625	-2.8283	158	C	26.6009	-0.8918	-1.7903
69	C	-10.7944	3.0097	-0.6749	114	S	66.0491	-0.1803	-3.5645	159	C	25.4775	-0.1674	-1.3709
70	C	-13.1754	-3.4035	1.7054	115	C	60.7358	0.4008	-3.0923	160	C	25.6547	1.0907	-0.7232
71	H	13.6780	2.8132	-2.3887	116	C	59.8799	1.3200	-2.5547	161	C	29.4125	1.2543	-0.7929
72	H	10.3122	-4.0254	0.5933	117	S	60.7591	2.6848	-1.8382	162	C	30.2747	0.3258	-1.3069
73	H	10.0665	-2.4810	1.4499	118	C	47.9336	-0.0280	-2.5437	163	S	29.4038	-1.0693	-1.9716
74	H	18.5458	2.6276	0.3850	119	C	47.0799	0.9018	-2.0129	164	C	33.6991	1.9018	-1.4599
75	H	18.0006	-1.7926	-1.9431	120	S	47.9529	2.2756	-1.2992	165	C	32.3248	1.7234	-1.4081
76	H	21.2700	2.2095	0.0603	121	C	45.6804	0.8704	-1.9817	166	C	31.7334	0.4504	-1.3861
77	H	15.2761	-1.3677	-1.6178	122	C	50.7539	2.0887	-1.4913	167	C	34.5736	0.7978	-1.5131
78	H	2.4635	-1.8599	-1.0136	123	C	51.8733	1.3629	-1.9227	168	C	33.9824	-0.4752	-1.4913
79	H	5.7499	2.1269	1.0098	124	C	51.6929	0.1156	-2.5878	169	C	32.6081	-0.6536	-1.4390
80	H	5.1980	-2.2844	-1.3341	125	C	50.4364	-0.4161	-2.8306	170	O	34.2015	3.1843	-1.4374
81	H	8.4720	1.6985	0.6858	126	C	49.3149	0.3105	-2.4052	171	O	32.1060	-1.9362	-1.4610
82	H	10.4253	2.1538	-0.3999	127	C	49.4975	1.5589	-1.7370	172	C	34.2944	3.8191	-2.7193
83	H	13.3204	-1.8210	-0.5377	128	C	53.2580	1.6936	-1.7875	173	C	32.0154	-2.5713	-0.1790
84	H	-8.5785	-1.7583	-0.6378	129	C	54.1155	0.7663	-2.3112	174	H	58.8562	3.6788	-4.3132
85	H	-5.2789	2.1759	1.4349	130	S	53.2379	-0.6127	-3.0009	175	H	55.4100	-3.1496	-1.4187
86	H	-5.8584	-2.2076	-0.9541	131	C	57.5532	2.3168	-2.4218	176	H	55.1751	-1.6138	-0.5437
87	H	-2.5473	1.7344	1.1162	132	C	56.1773	2.1489	-2.3801	177	H	63.6854	3.4243	-1.4772
88	H	-21.4108	-2.1018	-0.1540	133	C	55.5756	0.8805	-2.3812	178	H	63.1176	-0.9335	-3.9132
89	H	-22.9542	-0.2921	0.9223	134	C	58.4191	1.2066	-2.4871	179	H	66.4297	2.9828	-1.7888
90	H	-18.0851	1.7844	2.0041	135	C	57.8176	-0.0615	-2.4889	180	H	67.9793	1.1703	-2.8515
91	H	-18.6680	-2.5513	-0.4674	136	C	56.4415	-0.2294	-2.4475	181	H	60.3937	-0.4913	-3.6005
92	H	-15.3628	1.3345	1.6892	137	O	58.0645	3.5953	-2.3775	182	H	47.5796	-0.9320	-3.0208
93	H	-13.3989	1.7976	0.6039	138	O	55.9285	-1.5073	-2.4930	183	H	50.8776	3.0375	-0.9822
94	H	-10.5457	-2.2055	0.4207	139	C	44.4670	0.8618	-1.9427	184	H	50.3127	-1.3667	-3.3364
95	H	-10.3678	3.9910	-0.4720	140	C	36.8939	-0.0045	-2.1099	185	H	53.5991	2.5951	-1.2957
96	H	-10.1387	2.4607	-1.3580	141	C	36.0324	0.9222	-1.5918	186	H	55.5641	3.0410	-2.3577
97	H	-13.6026	-4.3849	1.5044	142	S	36.9033	2.3140	-0.9199	187	H	58.4319	-0.9529	-2.5117
98	H	-13.8417	-2.8447	2.3701	143	C	39.7056	2.1336	-1.0982	188	H	36.5568	-0.9133	-2.5909
99	H	13.4326	4.3579	-1.5326	144	C	40.8302	1.4095	-1.5197	189	H	39.8251	3.0897	-0.6019

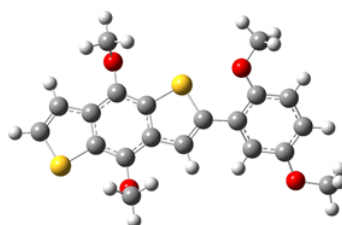
continues



## D<sub>2</sub> geometry continuation

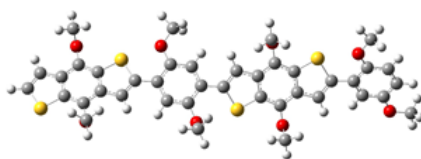
190	H	39.2797	-1.3406	-2.9112	196	H	31.7042	2.6106	-1.3959	202	H	58.6112	5.2242	-3.4583
191	H	42.5602	2.6669	-0.9192	197	H	34.6031	-1.3623	-1.5036	203	H	57.2080	4.3477	-4.1282
192	H	23.7578	-1.4317	-1.9602	198	H	34.7093	4.8102	-2.5416	204	H	56.8220	-2.2740	-0.7667
193	H	27.0243	2.5920	0.0040	199	H	34.9573	3.2602	-3.3874	205	H	33.3050	3.9116	-3.1790
194	H	26.4825	-1.8508	-2.2814	200	H	31.6003	-3.5623	-0.3563	206	H	33.0056	-2.6639	0.2788
195	H	29.7489	2.1657	-0.3163	201	H	31.3536	-2.0126	0.4903					

## 13) E<sub>1</sub>



1	C	-1.9928	1.1391	-2.7954	16	C	-9.0540	7.3689	-6.8937	31	C	-4.9141	3.4728	0.2317
2	H	-1.8891	1.0972	-3.8785	17	S	-8.8330	8.1340	-5.3326	32	C	-4.3015	2.8872	1.3413
3	H	-1.0408	1.4530	-2.3532	18	O	-7.3798	7.6347	-2.5940	33	O	-3.0188	2.0870	-2.5425
4	H	-2.2631	0.1473	-2.4170	19	O	-6.7446	3.7114	-6.5565	34	O	-4.8295	3.2274	2.5579
5	C	-4.2660	2.6428	3.7221	20	H	-8.4480	5.5659	-7.9009	35	H	-1.9733	1.0467	-0.2784
6	H	-4.8345	3.0408	4.5612	21	H	-9.6805	7.8546	-7.6271	36	H	-5.7640	4.1194	0.4066
7	H	-3.2110	2.9162	3.8387	22	C	-5.7863	5.1197	-2.1099	37	C	-5.6446	3.9146	-7.4530
8	H	-4.3592	1.5509	3.7079	23	C	-5.1536	3.9108	-2.1881	38	H	-4.6941	3.9304	-6.9101
9	C	-6.8874	4.6864	-5.5937	24	S	-5.3351	3.1835	-3.7966	39	H	-5.6548	3.0732	-8.1453
10	C	-7.6659	5.8282	-5.8331	25	H	-5.7912	5.7247	-1.2143	40	H	-5.7593	4.8500	-8.0105
11	C	-7.8042	6.8074	-4.8093	26	H	-2.7433	1.5303	1.9843	41	C	-6.3296	8.6076	-2.5065
12	C	-7.1986	6.6764	-3.5655	27	C	-3.4062	2.3186	-1.2530	42	H	-5.3724	8.1341	-2.2660
13	C	-6.4567	5.5117	-3.3126	28	C	-2.8002	1.7313	-0.1479	43	H	-6.2337	9.1643	-3.4442
14	C	-6.3127	4.5353	-4.3365	29	C	-3.2376	2.0104	1.1508	44	H	-6.6114	9.2898	-1.7050
15	C	-8.4028	6.1867	-7.0168	30	C	-4.4834	3.2218	-1.0733					

## 14) E<sub>2</sub>



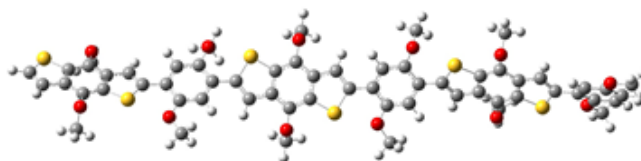
1	C	-3.5812	1.6723	-3.1090	11	S	5.8216	1.3435	0.6611	21	C	-2.3289	2.4075	1.4656
2	C	-4.0324	1.8057	4.0555	12	O	3.0800	1.2926	2.1987	22	C	-3.6545	2.5645	1.8439
3	C	2.9194	1.8363	-1.9982	13	O	2.8613	2.0346	-3.3597	23	O	-2.6036	1.7308	-2.0792
4	C	4.1500	1.6814	-1.3438	14	C	0.4772	1.7079	0.7455	24	O	-3.9351	2.9092	3.1502
5	C	4.1736	1.4917	0.0664	15	C	-0.5228	1.9230	-0.1645	25	C	2.7927	0.8294	-4.1330
6	C	3.0164	1.4578	0.8337	16	S	0.1249	2.0481	-1.8162	26	C	2.9438	-0.0646	2.6417
7	C	1.7881	1.6501	0.1808	17	C	-2.9871	1.9910	-0.7989	27	C	-16.2338	0.8191	0.7547
8	C	1.7620	1.8337	-1.2282	18	C	-4.3145	2.1627	-0.4250	28	C	-17.6012	7.0075	3.8670
9	C	5.4763	1.7015	-1.9014	19	C	-4.6901	2.4338	0.9034	29	C	-9.7101	2.0190	0.5598
10	C	6.4423	1.5301	-0.9682	20	C	-1.9441	2.1015	0.1538	30	C	-8.4463	2.3982	1.0389

continues

## E<sub>2</sub> geometry continuation

31	C	-8.3493	3.2712	2.1573	50	O	-16.2820	6.5442	3.6280	69	H	3.0257	-0.0409	3.7279
32	C	-9.4713	3.7770	2.8006	51	C	-9.9027	-0.2108	-0.2013	70	H	-15.7219	-0.0294	0.3039
33	C	-10.7353	3.4311	2.2952	52	C	-9.3798	4.0021	5.1527	71	H	-16.8570	0.4666	1.5842
34	C	-10.8322	2.5524	1.1814	53	H	-3.0296	1.4751	-4.0264	72	H	-16.8668	1.3029	0.0026
35	C	-7.1569	2.0309	0.5428	54	H	-4.2957	0.8607	-2.9343	73	H	-17.4942	7.9854	4.3339
36	C	-6.1115	2.5774	1.2346	55	H	-4.1189	2.6212	-3.2043	74	H	-18.1460	6.3416	4.5466
37	S	-6.6754	3.5945	2.5776	56	H	-4.2498	2.2290	5.0355	75	H	-18.1668	7.1136	2.9339
38	O	-9.3450	4.6375	3.8681	57	H	-3.0888	1.2510	4.0978	76	H	-7.0285	1.3782	-0.3093
39	O	-9.8287	1.1828	-0.5293	58	H	-4.8408	1.1272	3.7638	77	H	-12.1498	4.5466	3.5683
40	C	-12.0229	3.8627	2.7414	59	H	5.6760	1.8591	-2.9521	78	H	-18.2001	4.7535	2.8029
41	C	-13.0692	3.3520	2.0246	60	H	7.5111	1.5148	-1.1207	79	H	-17.6890	2.6211	1.7358
42	S	-12.5042	2.2623	0.7398	61	H	0.3038	1.6035	1.8067	80	H	-14.0230	5.6242	3.0762
43	C	-15.5559	2.8684	1.8062	62	H	-5.0887	2.1158	-1.1763	81	H	-10.7686	-0.4218	0.4341
44	C	-16.8701	3.2615	2.0331	63	H	-1.5764	2.5657	2.2269	82	H	-10.0083	-0.7427	-1.1466
45	C	-17.1651	4.4815	2.6475	64	H	1.8972	0.2511	-3.8836	83	H	-8.9913	-0.5442	0.3065
46	C	-14.4853	3.7093	2.2022	65	H	2.7466	1.1381	-5.1770	84	H	-10.3342	3.4900	5.3136
47	C	-14.8060	4.9314	2.7985	66	H	3.6803	0.2081	-3.9739	85	H	-8.5607	3.2835	5.2584
48	C	-16.1252	5.3228	3.0333	67	H	1.9703	-0.4763	2.3560	86	H	-9.2634	4.7962	5.8897
49	O	-15.2101	1.6892	1.2106	68	H	3.7381	-0.6952	2.2297					

## 15) E<sub>3</sub>



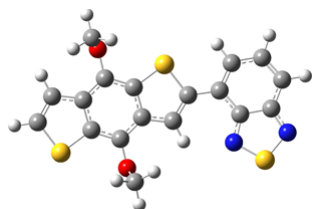
1	C	6.5248	-5.0996	11.5607	21	C	11.1673	-6.2711	11.8960	41	C	11.0187	-0.7753	2.6037
2	C	13.6652	-4.7438	10.7560	22	C	11.4598	-5.6099	10.7111	42	S	9.7721	-0.2672	3.7650
3	C	8.0771	-9.0860	16.6093	23	O	7.6147	-5.6822	12.2624	43	C	10.5869	1.0239	0.8570
4	C	8.8080	-9.6122	17.6843	24	O	12.7406	-5.6853	10.2037	44	C	10.7218	1.4798	-0.4485
5	C	10.2006	-9.3371	17.7854	25	C	5.8752	-8.4069	17.1390	45	C	11.3883	0.7335	-1.4380
6	C	10.8776	-8.5647	16.8501	26	C	12.5705	-7.1297	17.6657	46	C	11.1107	-0.2348	1.2430
7	C	10.1514	-8.0713	15.7546	27	C	9.3285	2.9681	1.5071	47	C	11.7389	-0.9846	0.2408
8	C	8.7591	-8.3392	15.6557	28	C	13.9026	-1.3194	-2.0173	48	C	11.8854	-0.5251	-1.0608
9	C	8.3512	-10.4541	18.7581	29	C	9.7835	-1.6902	6.1881	49	O	9.9416	1.7271	1.8286
10	C	9.3392	-10.7886	19.6215	30	C	10.3485	-2.7101	6.9702	50	O	12.4726	-1.3509	-1.9970
11	S	10.9029	-10.1197	19.1946	31	C	11.4740	-3.4309	6.4837	51	C	9.0063	0.2104	7.3593
12	O	12.2298	-8.3356	16.9679	32	C	12.0396	-3.1688	5.2428	52	C	14.3941	-3.3250	5.0908
13	O	6.7315	-9.3447	16.4735	33	C	11.4473	-2.1782	4.4420	53	H	5.6444	-5.2982	12.1692
14	C	10.6224	-7.3047	14.6443	34	C	10.3281	-1.4511	4.9328	54	H	6.6538	-4.0173	11.4524
15	C	9.6574	-6.9862	13.7278	35	C	9.9366	-3.1793	8.2560	55	H	6.3954	-5.5548	10.5734
16	S	8.0684	-7.6158	14.2162	36	C	10.6973	-4.2020	8.7518	56	H	14.6209	-4.9265	10.2661
17	C	8.8666	-5.6227	11.7301	37	S	12.0064	-4.6449	7.6354	57	H	13.7749	-4.8901	11.8359
18	C	9.1554	-4.9712	10.5374	38	O	13.1155	-3.8965	4.7853	58	H	13.3448	-3.7152	10.5595
19	C	10.4567	-4.9274	10.0033	39	O	8.6873	-0.9854	6.6355	59	H	7.3307	-10.7989	18.8489
20	C	9.8842	-6.2895	12.4564	40	C	11.8055	-1.7685	3.1216	60	H	9.2647	-11.4132	20.4991

continues

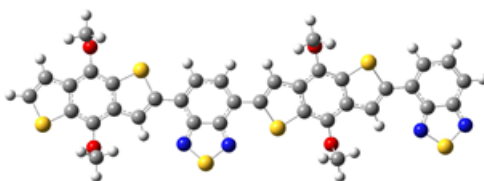
### E<sub>3</sub> geometry continuation

61	H	11.6586	-7.0170	14.5402	84	H	14.5398	-3.2392	6.1724	107	C	10.6367	4.5821	-12.7572
62	H	8.3572	-4.5036	9.9805	85	H	15.1393	-4.0043	4.6779	108	O	12.2752	7.0620	-9.8368
63	H	11.9698	-6.8204	12.3709	86	C	12.6604	8.3939	-10.1375	109	O	10.0722	3.6721	-13.6077
64	H	6.0200	-7.3946	16.7482	87	C	9.8766	4.0519	-14.9604	110	C	12.7181	5.8586	-4.1719
65	H	4.8541	-8.7307	16.9398	88	C	11.5259	4.0962	-5.2012	111	C	13.0238	0.0225	-7.7127
66	H	6.0550	-8.4069	18.2192	89	C	11.5445	2.8627	-4.5314	112	H	13.0226	8.8157	-9.2015
67	H	12.1801	-6.2496	17.1443	90	C	11.6160	1.6554	-5.2795	113	H	13.4653	8.4192	-10.8807
68	H	12.1844	-7.1446	18.6899	91	C	11.6589	1.6467	-6.6677	114	H	11.8119	8.9857	-10.4984
69	H	13.6591	-7.0874	17.6889	92	C	11.5960	2.8787	-7.3390	115	H	9.4162	3.1939	-15.4477
70	H	8.8675	3.3154	2.4299	93	C	11.5345	4.0863	-6.5904	116	H	10.8269	4.2809	-15.4570
71	H	10.0684	3.7031	1.1727	94	C	11.4853	2.6097	-3.1257	117	H	9.2072	4.9161	-15.0441
72	H	8.5583	2.8466	0.7384	95	C	11.5157	1.2840	-2.7912	118	H	11.4173	3.4050	-2.3969
73	H	14.2153	-2.0155	-2.7947	96	S	11.6358	0.2482	-4.2294	119	H	11.5878	2.3313	-9.4768
74	H	14.3148	-1.6388	-1.0540	97	O	11.7037	0.4603	-7.3651	120	H	10.9501	6.2266	-14.1280
75	H	14.2714	-0.3161	-2.2557	98	O	11.4481	5.2784	-4.4971	121	H	11.9144	7.6956	-12.4371
76	H	9.0910	-2.7589	8.7817	99	C	11.5659	3.1275	-8.7466	122	H	10.4121	3.1767	-11.1792
77	H	12.6241	-2.2207	2.5804	100	C	11.4906	4.4499	-9.0841	123	H	13.2901	6.0899	-5.0760
78	H	10.2802	2.4240	-0.7303	101	S	11.4757	5.4879	-7.6425	124	H	12.5043	6.7811	-3.6324
79	H	12.0989	-1.9814	0.4600	102	C	11.7472	6.2833	-10.8265	125	H	13.3046	5.1888	-3.5340
80	H	9.5729	0.9099	6.7365	103	C	11.6007	6.7033	-12.1438	126	H	13.5230	0.7506	-8.3604
81	H	8.0548	0.6624	7.6384	104	C	11.0516	5.8618	-13.1151	127	H	13.6321	-0.1431	-6.8176
82	H	9.5821	-0.0184	8.2623	105	C	11.3397	4.9791	-10.4486	128	H	12.9025	-0.9188	-8.2480
83	H	14.5037	-2.3369	4.6314	106	C	10.7778	4.1627	-11.4331					

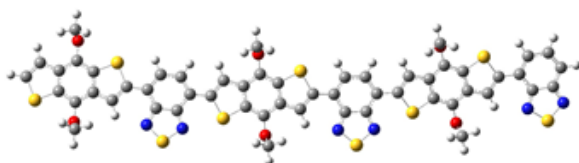
### 16) F<sub>1</sub>



1	C	-6.3838	4.5107	-5.2528	14	C	-5.3842	5.0217	-1.7441	27	C	-2.7131	3.2206	1.4673
2	C	-7.2882	5.5593	-5.4855	15	C	-4.6158	3.8940	-1.8312	28	C	-3.5232	3.8972	0.4665
3	C	-7.5498	6.4999	-4.4506	16	S	-4.7070	3.1623	-3.4520	29	C	-3.8044	3.2588	-0.7982
4	C	-6.9488	6.4224	-3.1993	17	H	-5.4718	5.5919	-0.8330	30	C	-3.2541	2.0011	-0.9686
5	C	-6.0745	5.3507	-2.9546	18	C	-5.0758	3.9177	-7.1355	31	C	-2.4607	1.3483	0.0156
6	C	-5.8079	4.4153	-3.9930	19	H	-4.1263	4.0595	-6.6095	32	N	-2.5367	3.9345	2.5830
7	C	-8.0495	5.8475	-6.6717	20	H	-4.9863	3.0834	-7.8303	33	S	-3.3354	5.3489	2.3705
8	C	-8.8344	6.9452	-6.5378	21	H	-5.3250	4.8300	-7.6867	34	N	-3.9290	5.1065	0.8596
9	S	-8.7183	7.7067	-4.9658	22	C	-6.2970	8.3756	-2.0209	35	H	-1.5826	1.4373	1.9808
10	O	-7.2656	7.3360	-2.2241	23	H	-5.3333	7.9639	-1.7073	36	H	-3.4390	1.4678	-1.8937
11	O	-6.1223	3.5667	-6.2192	24	H	-6.1636	8.9650	-2.9337	37	H	-2.0761	0.3605	-0.2109
12	H	-8.0146	5.2401	-7.5654	25	H	-6.6962	9.0111	-1.2313					
13	H	-9.5061	7.3657	-7.2716	26	C	-2.1817	1.9259	1.2236					

17) F<sub>2</sub>

1	C	-8.7516	1.7464	-0.4301	25	H	-8.4582	-4.0828	1.1322	49	S	6.7148	2.2546	0.2212
2	C	-9.9244	0.9757	-0.4841	26	C	-0.7731	0.0540	0.0618	50	C	3.6491	3.5399	1.9349
3	C	-9.8379	-0.4385	-0.3536	27	C	-1.5653	-1.1212	0.2955	51	C	6.8968	-0.3162	-0.2185
4	C	-8.6288	-1.1021	-0.1798	28	C	-3.0214	-1.0836	0.2501	52	C	4.9880	-3.0964	0.7301
5	C	-7.4526	-0.3338	-0.1654	29	C	-3.7221	0.1426	-0.0348	53	C	7.6846	0.7955	-0.0975
6	C	-7.5415	1.0810	-0.2888	30	C	-2.9075	1.2411	-0.2597	54	H	4.5851	3.3136	2.4549
7	C	-11.2821	1.4109	-0.6743	31	C	-1.4967	1.1993	-0.2221	55	H	3.4793	4.6161	1.9424
8	C	-12.1668	0.3831	-0.6810	32	N	-1.0806	-2.3314	0.5741	56	H	2.8208	3.0333	2.4407
9	S	-11.4235	-1.1873	-0.4667	33	S	-2.3584	-3.3372	0.7575	57	H	7.3037	-1.2919	-0.4312
10	O	-8.5996	-2.4724	-0.0938	34	N	-3.5765	-2.2713	0.4996	58	H	5.9275	-2.7549	1.1747
11	O	-8.7888	3.1140	-0.5763	35	H	-3.3647	2.1930	-0.5033	59	H	4.1948	-3.0699	1.4840
12	H	-11.5629	2.4448	-0.8192	36	H	-0.9652	2.1140	-0.4532	60	H	5.1073	-4.1144	0.3617
13	H	-13.2369	0.4383	-0.8161	37	C	0.6858	0.0656	0.1169	61	C	9.1341	0.9057	-0.2171
14	C	-6.0973	-0.7809	-0.0602	38	C	1.4740	1.1747	0.2893	62	C	9.9963	-0.2517	-0.2706
15	C	-5.1737	0.2286	-0.0955	39	S	1.6567	-1.3987	-0.1244	63	C	9.7727	2.1312	-0.2875
16	S	-5.9525	1.8220	-0.2646	40	C	2.8740	0.9111	0.2161	64	C	11.4365	-0.0904	-0.3945
17	H	-5.8151	-1.8187	0.0164	41	H	1.0768	2.1648	0.4626	65	N	9.6217	-1.5314	-0.2091
18	C	-9.0125	3.8429	0.6390	42	C	3.1375	-0.4663	-0.0227	66	C	11.1826	2.2788	-0.4067
19	H	-8.2133	3.6523	1.3623	43	C	3.9460	1.8134	0.3422	67	H	9.1770	3.0361	-0.2633
20	H	-9.0133	4.8977	0.3663	44	C	4.4284	-0.9660	-0.1472	68	C	12.0235	1.2014	-0.4639
21	H	-9.9764	3.5782	1.0852	45	C	5.2316	1.3189	0.1807	69	N	12.1024	-1.2484	-0.4282
22	C	-8.4578	-2.9983	1.2343	46	O	3.7216	3.1543	0.5544	70	S	10.9846	-2.4401	-0.3096
23	H	-7.5182	-2.6736	1.6906	47	C	5.4979	-0.0583	-0.0650	71	H	11.5888	3.2825	-0.4578
24	H	-9.2970	-2.6886	1.8652	48	O	4.6334	-2.2985	-0.4095	72	H	13.0967	1.3021	-0.5582

18) F<sub>3</sub>

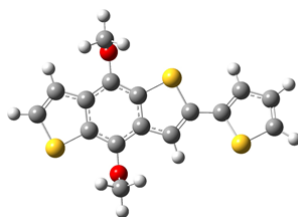
1	C	-15.0102	2.2156	-0.7587	11	O	-14.9365	3.5771	-0.9409	21	C	-9.2328	1.2574	-0.3614
2	C	-16.2390	1.5386	-0.8198	12	C	-12.5790	-0.5012	-0.2426	22	C	-7.8333	1.1061	-0.2653
3	C	-16.2693	0.1274	-0.6460	13	C	-11.5767	0.4297	-0.2759	23	N	-7.7284	-2.4390	0.5581
4	C	-15.1220	-0.6249	-0.4238	14	S	-12.2199	2.0751	-0.5151	24	S	-9.0864	-3.3416	0.6909
5	C	-13.8898	0.0489	-0.3972	15	C	-15.1229	4.3510	0.2527	25	N	-10.2052	-2.1859	0.3802
6	C	-13.8618	1.4614	-0.5629	16	C	-15.1590	-2.4735	1.0572	26	C	-5.7616	-0.1936	0.1717
7	C	-17.5514	2.0739	-1.0611	17	C	-7.2124	-0.0891	0.0552	27	C	-4.8865	0.8564	0.2895
8	C	-18.5146	1.1208	-1.0617	18	C	-8.1049	-1.1963	0.2600	28	S	-4.9110	-1.7504	0.1043
9	S	-17.9059	-0.4972	-0.7809	19	C	-9.5500	-1.0462	0.1538	29	C	-3.5148	0.4727	0.3132
10	O	-15.2027	-1.9892	-0.2934	20	C	-10.1405	0.2292	-0.1634	30	C	-3.3616	-0.9371	0.2058

continues

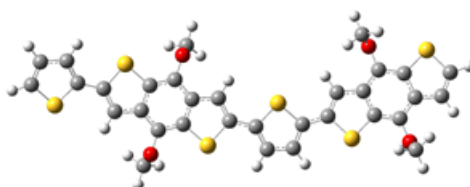
### F<sub>3</sub> geometry continuation

31	C	-2.3759	1.2928	0.4152	57	H	-14.2111	-2.2163	1.5393	83	C	13.3365	-0.0175	-0.4805
32	C	-2.1149	-1.5496	0.1881	58	H	-15.9892	-2.0678	1.6442	84	C	14.0842	1.1045	-0.2523
33	C	-1.1327	0.6819	0.3659	59	H	-15.2527	-3.5569	0.9935	85	S	13.0697	2.4715	0.2752
34	O	-2.4958	2.6602	0.5057	60	H	-9.6038	2.2407	-0.6253	86	C	10.0463	3.3947	2.2505
35	C	-0.9758	-0.7287	0.2510	61	H	-7.2250	1.9765	-0.4755	87	C	11.5718	-2.9743	0.2142
36	O	-2.0107	-2.9124	0.0555	62	H	-5.1983	1.8891	0.3532	88	C	18.3866	1.7394	-0.7008
37	S	0.4222	1.4930	0.4035	63	H	-1.6828	2.9110	2.4201	89	C	17.8465	0.4324	-0.8345
38	C	-2.5799	3.1646	1.8468	64	H	-2.6620	4.2475	1.7605	90	C	16.4195	0.1946	-0.6891
39	C	0.3983	-1.1142	0.1914	65	H	-3.4623	2.7693	2.3605	91	C	15.5221	1.2909	-0.4063
40	C	-1.8060	-3.6260	1.2841	66	H	0.7263	-2.1352	0.0800	92	C	16.1165	2.5343	-0.2882
41	C	1.2761	-0.0661	0.2641	67	H	-0.8664	-3.3301	1.7606	93	C	17.5140	2.7565	-0.4304
42	C	2.7291	-0.0874	0.2244	68	H	-2.6364	-3.4572	1.9769	94	N	18.5487	-0.6742	-1.0927
43	C	3.4955	-1.3076	0.2275	69	H	-1.7626	-4.6813	1.0179	95	S	17.4780	-1.9111	-1.1438
44	C	3.4843	1.0738	0.1744	70	H	2.9748	2.0298	0.1470	96	N	16.0906	-1.0896	-0.8402
45	C	4.9515	-1.2770	0.1925	71	H	5.3711	2.0680	0.0611	97	H	7.4642	2.0959	0.7149
46	N	3.0062	-2.5480	0.2624	72	C	10.3299	1.8920	0.4459	98	H	13.7720	-0.9410	-0.8270
47	C	4.8941	1.0989	0.1328	73	C	9.2927	0.9606	0.2559	99	H	11.0194	3.1578	2.6916
48	C	5.6813	-0.0400	0.1543	74	C	9.6015	-0.3648	-0.1566	100	H	9.8269	4.4513	2.4002
49	N	5.5007	-2.4908	0.1996	75	C	10.9047	-0.7846	-0.3931	101	H	9.2727	2.7874	2.7315
50	S	4.2796	-3.5785	0.2444	76	C	11.9377	0.1555	-0.2414	102	H	12.5145	-2.6525	0.6673
51	H	-17.7420	3.1219	-1.2451	77	C	11.6263	1.4794	0.1793	103	H	10.8043	-3.0620	0.9896
52	H	-19.5731	1.2553	-1.2277	78	C	7.8892	1.1495	0.4127	104	H	11.7120	-3.9396	-0.2706
53	H	-12.3839	-1.5555	-0.1298	79	C	7.1385	0.0340	0.1405	105	H	19.4512	1.8948	-0.8138
54	H	-14.3572	4.1149	0.9984	80	S	8.1580	-1.3465	-0.3140	106	H	15.4931	3.3968	-0.0847
55	H	-15.0319	5.3954	-0.0439	81	O	11.1564	-2.0663	-0.8172	107	H	17.8838	3.7696	-0.3221
56	H	-16.1141	4.1777	0.6839	82	O	10.0573	3.1842	0.8307					

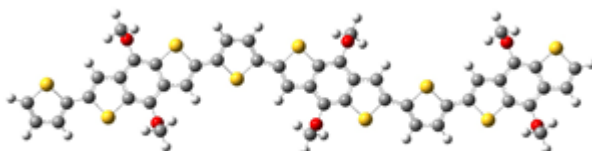
### 19) G1<sub>1</sub>



1	C	-6.1824	4.2869	-4.9305	12	C	-5.5282	4.6107	-1.3198	23	H	-9.1656	7.1951	-7.0809
2	C	-7.0829	5.3321	-5.1917	13	C	-4.7295	3.5061	-1.4024	24	H	-5.7409	5.1185	-0.3888
3	C	-7.4646	6.2050	-4.1352	14	S	-4.6435	2.8698	-3.0563	25	H	-3.7950	3.9530	-6.0809
4	C	-6.9814	6.0657	-2.8383	15	C	-4.6845	3.8232	-6.7054	26	H	-4.5080	3.0295	-7.4306
5	C	-6.1090	5.0000	-2.5708	16	C	-6.5410	8.0367	-1.6007	27	H	-5.5404	7.7115	-1.2987
6	C	-5.7258	4.1290	-3.6289	17	C	-2.8434	1.2260	0.8988	28	H	-6.4648	8.6654	-2.4934
7	C	-7.7346	5.6739	-6.4283	18	C	-2.8368	2.2580	1.7937	29	H	-2.3983	0.2609	1.1010
8	C	-8.5561	6.7457	-6.3109	19	S	-3.6308	3.6606	1.1592	30	H	-3.6254	0.8602	-1.1386
9	S	-8.6103	7.4153	-4.6933	20	C	-4.0006	2.8373	-0.3442	31	H	-2.4134	2.2857	2.7860
10	O	-7.3994	6.9116	-1.8375	21	C	-3.5030	1.5540	-0.3171	32	H	-4.8991	4.7593	-7.2306
11	O	-5.8078	3.4041	-5.9174	22	H	-7.5997	5.1202	-7.3470	33	H	-7.0001	8.6052	-0.7927

20) G1<sub>2</sub>

1	C	8.0836	-0.9596	0.0783	23	C	-3.1494	0.0695	-0.0972	45	H	4.0560	1.3035	-0.3156
2	C	8.9069	0.1734	-0.0274	24	C	-3.6228	-1.2709	-0.0351	46	H	8.0534	-2.6564	2.1419
3	C	8.3120	1.4600	-0.1495	25	C	-4.9730	-1.5860	0.0322	47	H	9.3483	-3.6492	1.4201
4	C	6.9341	1.6477	-0.1744	26	C	-5.8966	-0.5275	0.0698	48	H	5.2763	2.9901	1.4414
5	C	6.1129	0.5117	-0.1066	27	C	-5.4237	0.8128	0.0008	49	H	6.9152	3.6937	1.5440
6	C	6.7092	-0.7744	0.0202	28	C	-1.7213	0.1307	-0.1465	50	H	0.3632	-3.5409	-0.4675
7	C	10.3437	0.2458	-0.0497	29	C	-1.1132	-1.0948	-0.1219	51	H	2.9641	-3.4156	-0.4566
8	C	10.8042	1.5146	-0.1764	30	S	-2.2930	-2.4175	-0.0223	52	H	9.6962	-1.9812	1.9514
9	S	9.5340	2.7151	-0.2878	31	O	-5.3820	-2.8961	0.1230	53	H	5.6398	4.5330	0.6212
10	O	6.3994	2.9055	-0.3249	32	O	-3.6587	2.4372	-0.1384	54	H	-1.1741	1.0627	-0.1895
11	O	8.6161	-2.2246	0.1732	33	C	-7.3207	-0.5863	0.2034	55	H	-7.8633	-1.5143	0.3228
12	C	4.6848	0.4351	-0.1729	34	C	-7.9245	0.6395	0.2258	56	H	-4.3859	2.9391	-2.0359
13	C	4.1951	-0.8392	-0.0936	35	S	-6.7503	1.9605	0.0781	57	H	-3.1409	4.0009	-1.3251
14	S	5.4924	-2.0398	0.0715	36	C	-3.4572	2.9669	-1.4573	58	H	-6.6129	-2.9636	-1.5711
15	C	8.9446	-2.6410	1.5065	37	C	-5.7675	-3.4950	-1.1231	59	H	-4.9296	-3.5038	-1.8274
16	C	6.0395	3.5591	0.9013	38	C	-11.3410	2.0803	0.7725	60	H	-11.9700	2.9143	1.0537
17	C	0.9141	-2.6208	-0.3229	39	C	-11.8319	0.8554	0.4189	61	H	-9.3495	3.0163	1.0037
18	C	0.2976	-1.3996	-0.1522	40	S	-10.5616	-0.2545	0.0256	62	H	-12.8603	0.5334	0.3623
19	C	2.8202	-1.2788	-0.1398	41	C	-9.3323	0.9505	0.3607	63	H	-2.6801	2.4101	-1.9904
20	C	2.3258	-2.5532	-0.3157	42	C	-9.9210	2.1365	0.7383	64	H	-6.0602	-4.5184	-0.8913
21	S	1.5007	-0.1377	0.0454	43	H	10.9860	-0.6221	0.0052					
22	C	-4.0748	1.1269	-0.0999	44	H	11.8329	1.8390	-0.2296					

21) G1<sub>3</sub>

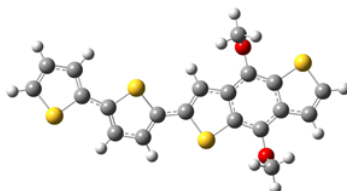
1	C	14.0295	-1.3143	0.1818	13	C	10.1645	-0.9774	-0.1403	25	C	0.9772	-1.2419	-0.1140
2	C	14.9153	-0.2260	0.1319	14	S	11.3866	-2.2507	0.0557	26	C	0.1094	-0.1366	-0.1097
3	C	14.3965	1.0923	0.0081	15	C	14.7132	-3.0590	1.6251	27	C	0.6489	1.1752	-0.2214
4	C	13.0335	1.3557	-0.0719	16	C	12.2208	3.2966	1.0111	28	C	4.3090	0.3029	-0.3523
5	C	12.1508	0.2651	-0.0538	17	C	6.8036	-2.5665	-0.5390	29	C	4.8546	-0.9497	-0.2927
6	C	12.6708	-1.0530	0.0741	18	C	6.2482	-1.3257	-0.3136	30	S	3.6111	-2.2087	-0.1479
7	C	16.3530	-0.2328	0.1679	19	C	8.7702	-1.3394	-0.2431	31	O	0.4987	-2.5242	0.0153
8	C	16.8862	1.0094	0.0820	20	C	8.2154	-2.5743	-0.4992	32	O	2.4947	2.7016	-0.4184
9	S	15.6887	2.2807	-0.0599	21	S	7.5085	-0.1425	-0.0171	33	C	-1.3132	-0.1203	0.0288
10	O	12.5722	2.6424	-0.2174	22	C	2.0108	1.4176	-0.3328	34	C	-1.8566	1.1347	0.0112
11	O	14.4907	-2.6062	0.2816	23	C	2.8806	0.3144	-0.3006	35	S	-0.6166	2.3915	-0.1755
12	C	10.7254	0.2681	-0.1808	24	C	2.3408	-0.9978	-0.1971	36	C	2.6972	3.1763	-1.7584

continues

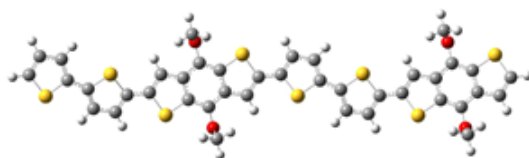
### G1<sub>3</sub> geometry continuation

37	C	0.1147	-3.1487	-1.2191	57	H	3.0757	4.1936	-1.6668	77	S	-12.6859	-2.0755	0.0679
38	C	-5.1901	2.7680	0.4527	58	H	-0.6972	-2.5973	-1.7037	78	C	-9.3777	-2.9270	1.6371
39	C	-5.7653	1.5374	0.2210	59	H	0.9651	-3.2193	-1.9044	79	C	-11.8801	3.4388	1.1654
40	S	-4.5249	0.3387	-0.0958	60	H	-5.7713	3.6528	0.6767	80	C	-17.2658	-2.3610	-0.6640
41	C	-3.2438	1.5154	0.1296	61	H	-3.1675	3.6300	0.5829	81	C	-17.8004	-1.1568	-0.3066
42	C	-3.7789	2.7559	0.4012	62	H	3.4295	2.5584	-2.2876	82	S	-16.5719	-0.0032	0.0942
43	H	16.9420	-1.1370	0.2330	63	H	-0.2282	-4.1496	-0.9598	83	C	-15.3006	-1.1616	-0.2467
44	H	17.9318	1.2789	0.0760	64	C	-10.0428	-1.1433	0.2328	84	C	-15.8455	-2.3658	-0.6296
45	H	10.1526	1.1720	-0.3373	65	C	-9.1568	-0.0531	0.2100	85	H	-7.1488	-0.9741	0.3193
46	H	13.7855	-3.0385	2.2055	66	C	-9.6776	1.2677	0.1215	86	H	-13.9179	1.3523	-0.2587
47	H	15.0701	-4.0852	1.5456	67	C	-11.0377	1.5327	0.0437	87	H	-10.3156	-2.9263	2.2011
48	H	11.4073	2.7692	1.5194	68	C	-11.9216	0.4408	0.0293	88	H	-9.0160	-3.9493	1.5336
49	H	13.0838	3.3642	1.6808	69	C	-11.4016	-0.8796	0.1267	89	H	-12.7039	2.8938	1.6370
50	H	6.2079	-3.4445	-0.7511	70	C	-7.7279	-0.0629	0.2558	90	H	-11.0342	3.4883	1.8582
51	H	8.8127	-3.4585	-0.6784	71	C	-7.1645	1.1821	0.2057	91	H	-17.8641	-3.2156	-0.9502
52	H	15.4684	-2.4457	2.1271	72	S	-8.3900	2.4606	0.0795	92	H	-15.2413	-3.2216	-0.9008
53	H	11.8919	4.2988	0.7389	73	O	-11.4955	2.8239	-0.0732	93	H	-18.8395	-0.8721	-0.2486
54	H	4.9009	1.2049	-0.4280	74	O	-9.5777	-2.4352	0.3032	94	H	-8.6334	-2.3266	2.1699
55	H	-1.8986	-1.0175	0.1765	75	C	-13.3453	0.4464	-0.1138	95	H	-12.2061	4.4478	0.9159
56	H	1.7570	3.1848	-2.3186	76	C	-13.9053	-0.7994	-0.1119					

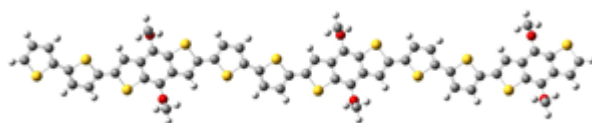
### 22) G2<sub>1</sub>



1	C	-6.4952	4.5594	-5.4399	15	C	-4.8874	3.7417	-1.9883	29	C	-1.9293	2.8493	4.7424
2	C	-7.3598	5.6434	-5.6634	16	S	-4.9250	3.0865	-3.6379	30	C	-1.0206	1.8515	4.5309
3	C	-7.6373	6.5457	-4.5992	17	H	-5.7611	5.4151	-0.9423	31	S	-1.0802	1.2673	2.9009
4	C	-7.0888	6.3966	-3.3299	18	C	-6.4684	8.3358	-2.1186	32	C	-2.3755	2.3773	2.4931
5	C	-6.2551	5.2920	-3.0974	19	H	-5.4840	7.9429	-1.8453	33	C	-2.7003	3.1491	3.5862
6	C	-5.9733	4.3935	-4.1645	20	H	-6.3765	8.9526	-3.0182	34	H	-2.0526	3.3488	5.6941
7	C	-8.0671	6.0014	-6.8642	21	H	-6.8606	8.9398	-1.3012	35	H	-0.3184	1.4214	5.2283
8	C	-8.8293	7.1124	-6.7141	22	C	-2.9544	1.4061	0.2058	36	H	-3.4866	3.8924	3.5657
9	S	-8.7555	7.8028	-5.1063	23	C	-2.9448	2.3964	1.1625	37	C	-5.1477	4.0183	-7.3110
10	O	-7.4113	7.2731	-2.3202	24	S	-3.7588	3.8278	0.5607	38	H	-4.2108	4.1353	-6.7572
11	O	-6.2192	3.6470	-6.4323	25	C	-4.1369	3.0500	-0.9657	39	H	-5.3756	4.9495	-7.8393
12	H	-8.0139	5.4304	-7.7808	26	C	-3.6202	1.7731	-0.9873	40	H	-5.0473	3.2056	-8.0296
13	H	-9.4619	7.5813	-7.4532	27	H	-2.5174	0.4296	0.3690					
14	C	-5.6260	4.8867	-1.8763	28	H	-3.7418	1.1057	-1.8305					

23) G2<sub>2</sub>

1	C	-5.4508	2.4111	-10.0020	27	H	-6.8653	3.0994	-12.4609	53	S	4.9031	-3.3267	4.7159
2	C	-6.5985	3.1800	-10.2540	28	H	-8.9954	4.5867	-12.1628	54	C	2.2070	1.4823	6.0795
3	C	-7.3012	3.7642	-9.1643	29	H	-5.6300	2.7432	-5.3825	55	C	7.0485	-4.5013	8.6553
4	C	-6.9010	3.6019	-7.8425	30	H	-6.1308	5.3954	-6.0130	56	C	6.8436	-3.4986	9.5760
5	C	-5.7726	2.8072	-7.5897	31	H	-7.2055	6.1751	-7.2080	57	S	5.7820	-2.2724	8.9119
6	C	-5.0681	2.2267	-8.6809	32	H	-7.8237	5.7648	-5.5861	58	C	5.5933	-3.1598	7.4104
7	C	-7.2283	3.4724	-11.5134	33	H	-1.0974	-1.0864	-4.0494	59	C	6.3499	-4.3102	7.4412
8	C	-8.3381	4.2377	-11.3806	34	H	-2.2117	-0.5300	-6.3388	60	C	7.6658	-2.7604	13.1565
9	S	-8.7112	4.6531	-9.7198	35	H	-2.2015	1.1252	1.5085	61	C	8.7806	-3.5280	12.9791
10	O	-7.6216	4.1608	-6.8137	36	H	-3.4444	1.5236	-0.7469	62	S	8.8864	-4.1392	11.3612
11	O	-4.7531	1.8122	-11.0250	37	H	-2.9990	2.9496	-10.9044	63	C	7.3788	-3.3631	10.9140
12	C	-5.2023	2.4419	-6.3291	38	H	-4.2043	3.5330	-12.0862	64	C	6.8675	-2.6662	11.9849
13	C	-4.1060	1.6324	-6.4324	39	H	-3.2865	2.0375	-12.4100	65	C	4.6312	-2.5006	1.0515
14	S	-3.7083	1.2650	-8.1238	40	C	3.1083	-2.2516	2.8451	66	H	1.5118	-1.7884	0.4695
15	C	-7.1575	5.4508	-6.3888	41	C	2.0379	-1.3811	2.5785	67	H	3.4889	-1.2120	7.3453
16	C	-1.7975	-0.2736	-4.1909	42	C	1.5354	-0.5533	3.6206	68	H	3.2474	1.3229	6.3799
17	C	-2.2146	0.5385	-3.1584	43	C	2.0588	-0.5668	4.9058	69	H	2.1815	2.0856	5.1666
18	S	-3.3655	1.7241	-3.7469	44	C	3.1088	-1.4594	5.1803	70	H	1.6732	2.0019	6.8743
19	C	-3.2984	1.0727	-5.3742	45	C	3.6130	-2.2853	4.1375	71	H	7.6615	-5.3686	8.8624
20	C	-2.4029	0.0271	-5.4311	46	C	1.3107	-1.2084	1.3599	72	H	6.3752	-5.0159	6.6212
21	C	-1.8109	0.8129	0.5489	47	C	0.3037	-0.2866	1.4423	73	H	7.4145	-2.2858	14.0957
22	C	-0.6245	0.1245	0.4163	48	S	0.1934	0.4318	3.0623	74	H	9.5501	-3.7735	13.6944
23	S	-0.3178	-0.2318	-1.2740	49	O	1.5267	0.2326	5.8900	75	H	5.9316	-2.1252	11.9374
24	C	-1.8251	0.5161	-1.7692	50	O	3.6079	-3.0844	1.8718	76	H	5.4949	-2.2024	1.6540
25	C	-2.4840	1.0306	-0.6735	51	C	3.7687	-1.7055	6.4246	77	H	4.2507	-1.6305	0.5071
26	C	-3.7545	2.6429	-11.6346	52	C	4.7439	-2.6615	6.3541	78	H	4.9303	-3.2722	0.3431

24) G2<sub>2</sub>

1	C	11.1754	-1.4023	0.8637	11	O	11.4250	-2.6935	1.2668	21	C	0.4689	1.6121	-0.9731
2	C	12.2204	-0.4865	0.6606	12	C	8.1783	0.5099	-0.0920	22	C	-0.2814	0.5286	-0.5704
3	C	11.9183	0.8325	0.2231	13	C	7.4302	-0.6057	0.1601	23	S	0.7706	-0.7837	-0.0713
4	C	10.6182	1.2604	-0.0218	14	S	8.4290	-1.9633	0.7194	24	C	2.2100	0.1397	-0.4607
5	C	9.5777	0.3351	0.1509	15	C	10.0636	3.4853	0.5619	25	C	1.8630	1.3943	-0.9137
6	C	9.8806	-0.9827	0.5931	16	C	3.8913	-1.7578	-0.2097	26	C	11.5173	-2.8697	2.6879
7	C	13.6363	-0.6870	0.8134	17	C	3.5229	-0.4318	-0.2819	27	C	-4.9093	-1.4727	-0.3284
8	C	14.3587	0.4191	0.5141	18	S	4.9313	0.5989	-0.1073	28	C	-3.8709	-0.5287	-0.4032
9	S	13.3804	1.7840	0.0139	19	C	6.0043	-0.7833	0.0158	29	C	-4.1906	0.8530	-0.5161
10	O	10.3689	2.5358	-0.4702	20	C	5.2800	-1.9539	-0.0411	30	C	-5.4973	1.3183	-0.5584

continues



G2<sub>3</sub> geometry continuation

31	C	-6.5352	0.3718	-0.5145	60	H	5.7432	-2.9307	0.0053	89	C	-24.0623	0.7259	0.0610
32	C	-6.2156	-1.0096	-0.3988	61	H	0.0236	2.5303	-1.3328	90	C	-24.8116	-0.4105	-0.0693
33	C	-2.4594	-0.7542	-0.4162	62	H	2.5958	2.1267	-1.2259	91	S	-23.7976	-1.8529	-0.2771
34	C	-1.7172	0.3899	-0.5201	63	H	10.5823	-2.5852	3.1809	92	C	-22.0070	3.1964	1.6133
35	S	-2.7403	1.8379	-0.6125	64	H	12.3406	-2.2813	3.1054	93	C	-28.4101	-1.3875	-0.3656
36	O	-5.7623	2.6606	-0.6932	65	H	11.7070	-3.9298	2.8517	94	C	-28.7324	-0.1568	0.1601
37	O	-4.6438	-2.8189	-0.2426	66	H	-2.0227	-1.7434	-0.3925	95	S	-27.2762	0.7427	0.5370
38	C	-7.9450	0.5894	-0.6049	67	H	-8.3795	1.5690	-0.7499	96	C	-26.2493	-0.5453	-0.0668
39	C	-8.6867	-0.5585	-0.5494	68	H	-6.8703	2.9457	1.0619	97	C	-27.0190	-1.6060	-0.4906
40	S	-7.6649	-2.0008	-0.3822	69	H	-5.1232	3.2910	1.1989	98	C	-31.7868	1.9281	0.7641
41	C	-5.9969	3.3525	0.5425	70	H	-6.1812	4.3931	0.2782	99	C	-32.4711	0.7533	0.8865
42	C	-12.2570	-1.6185	-0.8836	71	H	-12.9827	-2.3932	-1.0936	100	S	-31.4290	-0.6178	0.6955
43	C	-12.6128	-0.3066	-0.6550	72	H	-10.4103	-2.8062	-1.0513	101	C	-30.0376	0.4130	0.4191
44	S	-11.1823	0.6699	-0.3781	73	H	-16.1410	2.7997	-0.8117	102	C	-30.4043	1.7371	0.4976
45	C	-10.1207	-0.7057	-0.6204	74	H	-13.5729	2.3900	-0.9757	103	C	-20.5092	-3.4279	0.6656
46	C	-10.8627	-1.8416	-0.8624	75	H	-5.3361	-3.1448	1.7070	104	H	-18.1674	-1.5827	-0.6344
47	C	-15.6826	1.8279	-0.6840	76	H	-3.5852	-2.8214	1.5656	105	H	-24.4947	1.7129	0.1533
48	C	-16.4158	0.6821	-0.4632	77	H	-4.2554	-4.3757	1.0010	106	H	-22.8479	2.6886	2.0963
49	S	-15.3473	-0.7025	-0.3250	78	C	-21.0387	-1.3393	-0.3121	107	H	-21.0913	3.0014	2.1803
50	C	-13.9277	0.2859	-0.6155	79	C	-19.9971	-0.3972	-0.2639	108	H	-22.1961	4.2688	1.5845
51	C	-14.2906	1.6064	-0.7712	80	C	-20.3076	0.9769	-0.0660	109	H	-29.1585	-2.1016	-0.6830
52	C	-4.4448	-3.3069	1.0928	81	C	-21.6086	1.4368	0.0823	110	H	-26.5924	-2.5070	-0.9116
53	H	14.0750	-1.6287	1.1121	82	C	-22.6519	0.4988	0.0036	111	H	-32.2546	2.8999	0.8496
54	H	15.4324	0.5311	0.5365	83	C	-22.3413	-0.8757	-0.1921	112	H	-29.7049	2.5479	0.3410
55	H	7.7610	1.4278	-0.4830	84	C	-18.5927	-0.6111	-0.4228	113	H	-21.3600	-3.3982	1.3535
56	H	9.1572	3.1987	1.1048	85	C	-17.8461	0.5319	-0.3406	114	H	-19.6172	-3.0499	1.1753
57	H	10.8948	3.5794	1.2677	86	S	-18.8561	1.9648	-0.0596	115	H	-20.3378	-4.4540	0.3427
58	H	9.9025	4.4388	0.0603	87	O	-21.8660	2.7773	0.2475	116	H	-33.5220	0.6029	1.0791
59	H	3.1813	-2.5684	-0.3088	88	O	-20.7825	-2.6733	-0.5246					

**Figure S1:** Plots of the simulated absorption spectra, calculated at the TD-B3LYP/6-311G(d,p) level for the A-G oligomers.

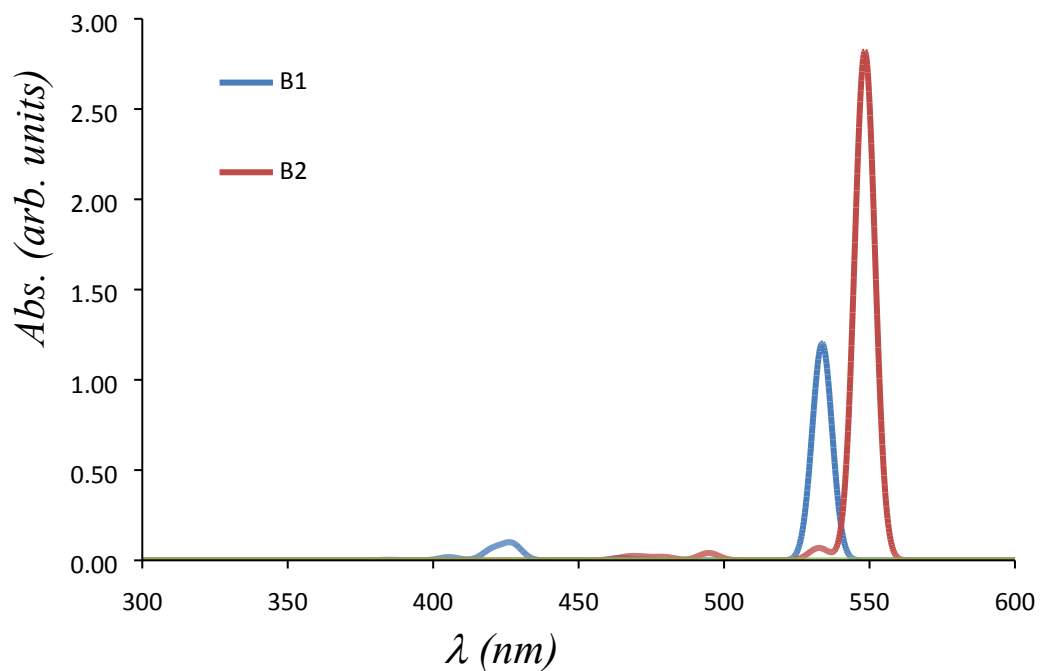
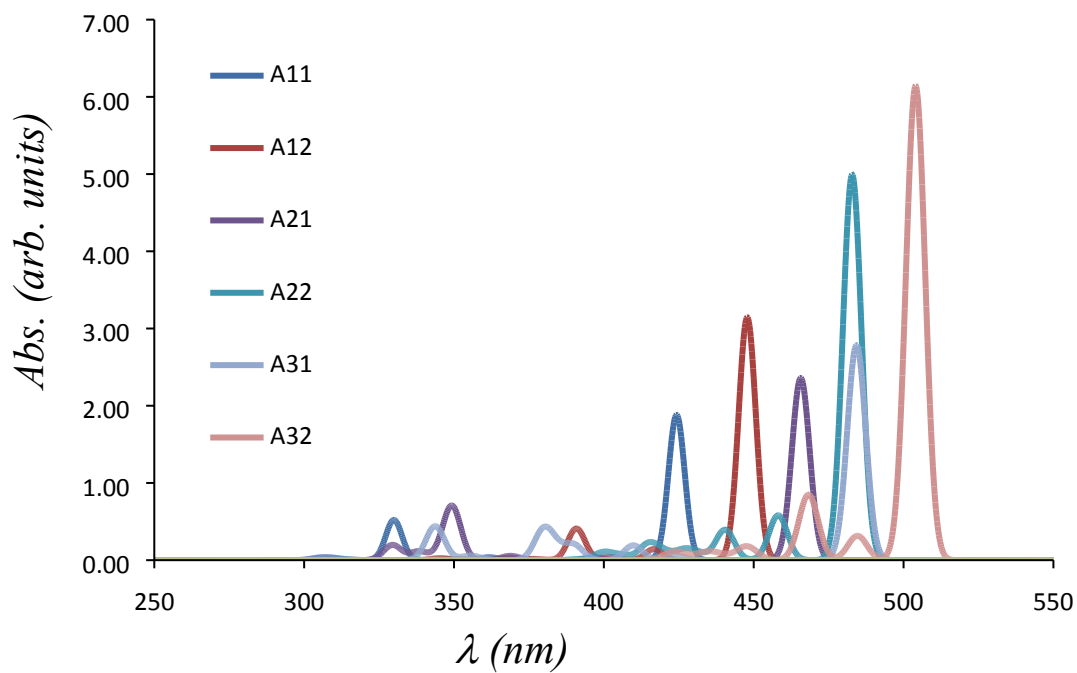


Figure S1: continue.

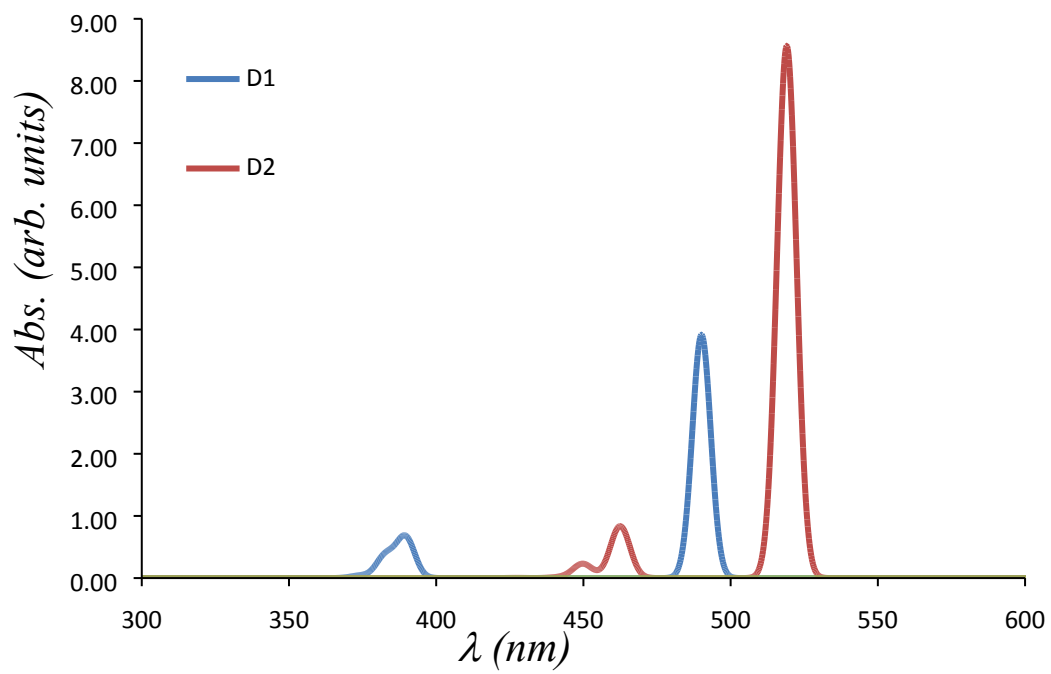
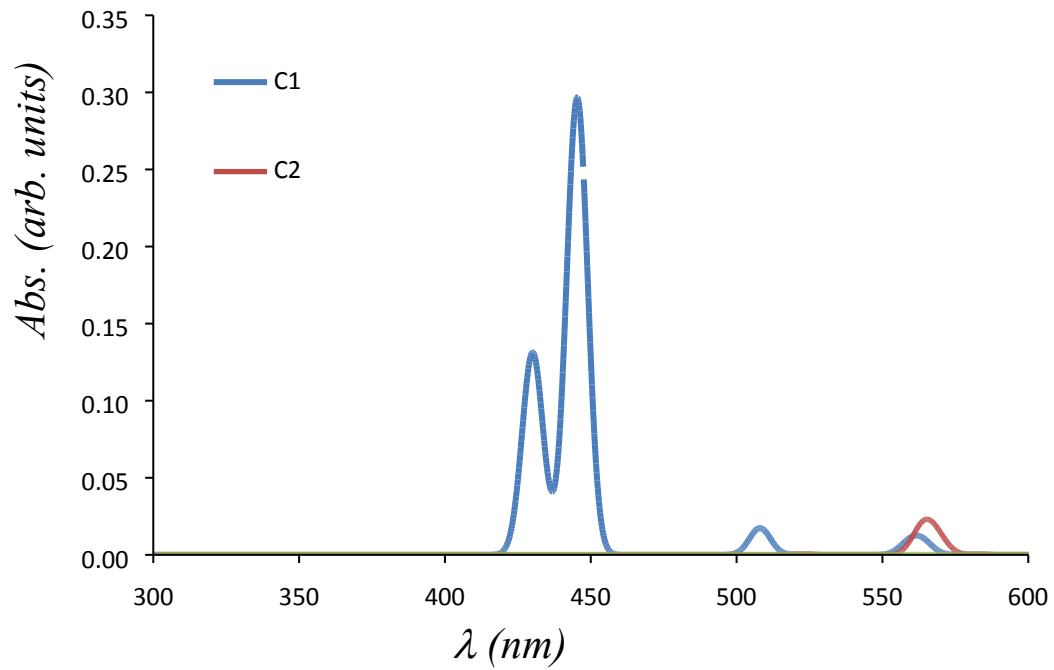


Figure S1: continue.

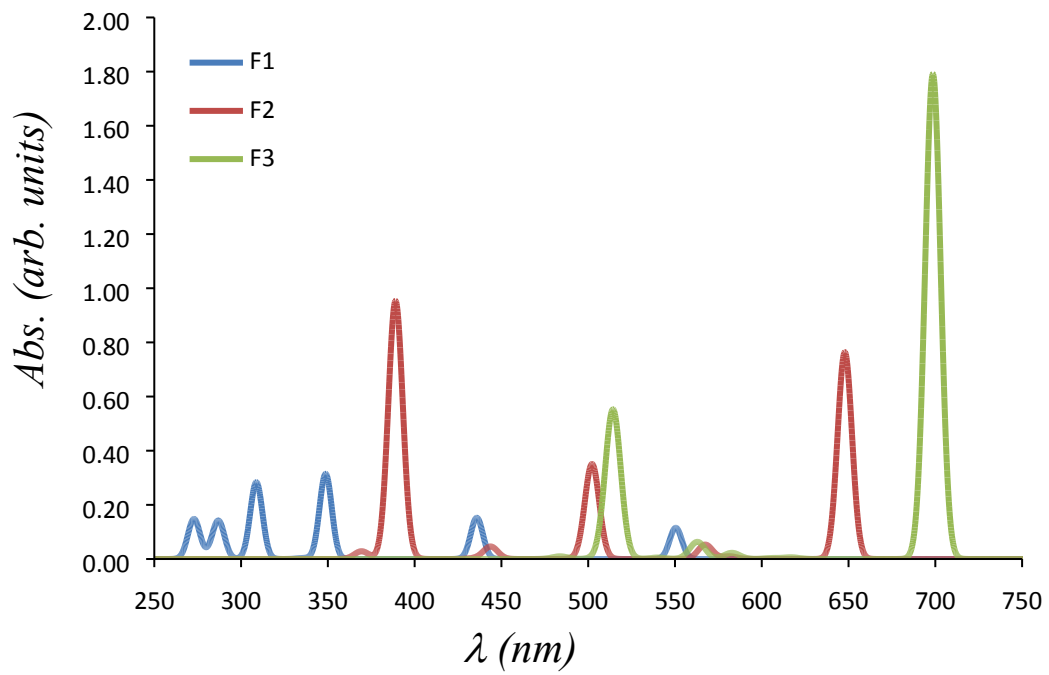
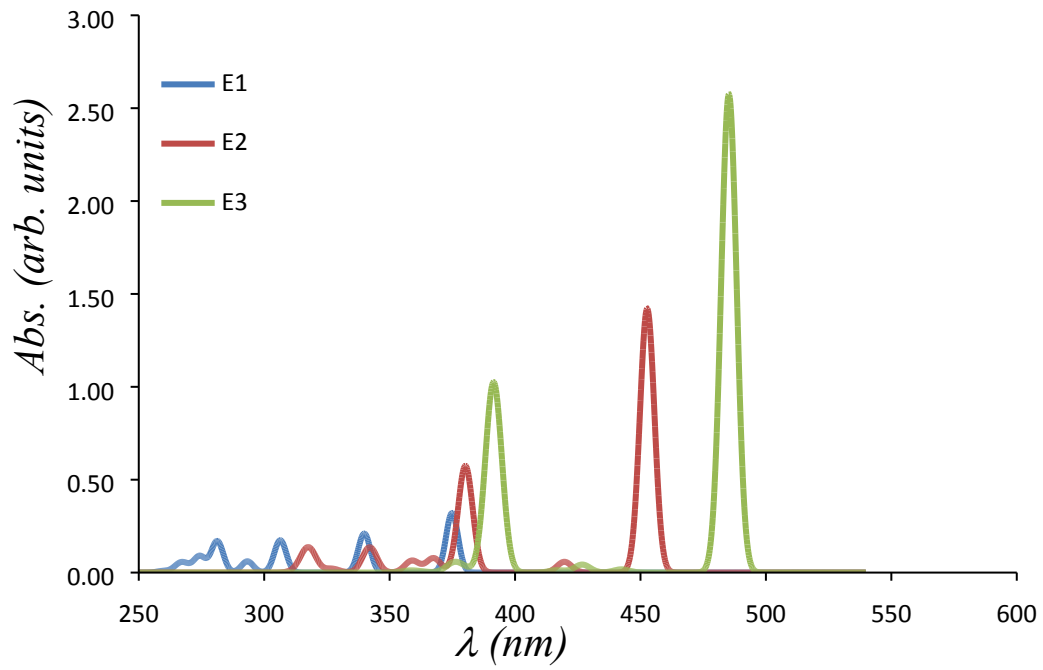


Figure S1: continue.

