

Supplementary data file

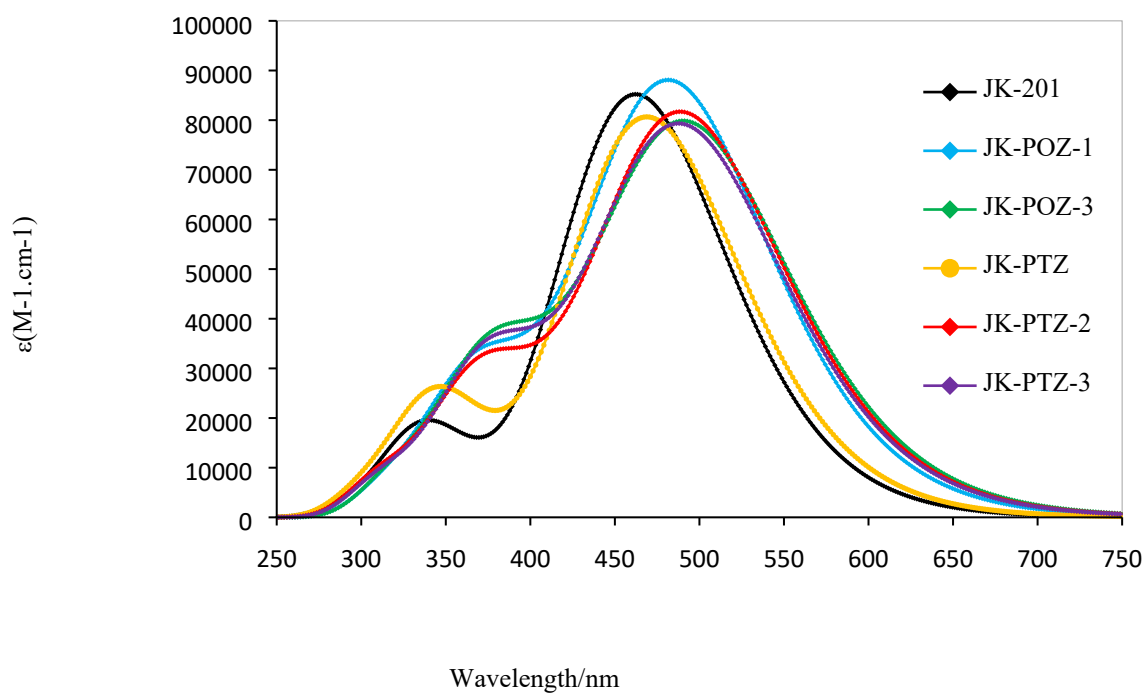
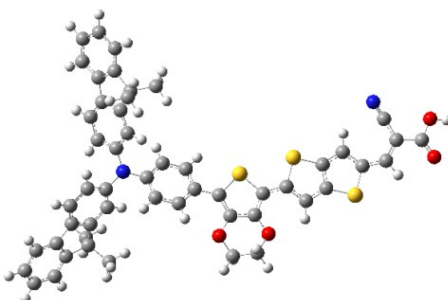


Fig. S1. Calculated absorption spectra of the reference and JK-POZ-1, JK-POZ-3, JK-PTZ, JK-PTZ-2 and JK-PTZ-3 designed dyes at PCM/LC-wPBE/6-31++G(d,p) level of theory in THF solvent.

The coordinate files for the molecular structures

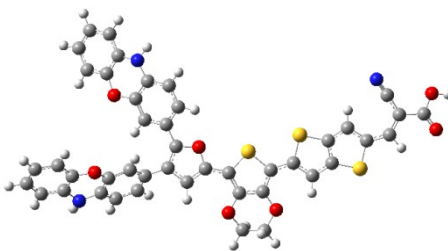
center Number	Atomic Number	Coordinates (Angstroms)			center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	1.886998	-1.24345	-0.7451	81	1	-7.85842	6.657864	1.149624
2	6	2.498433	-2.30476	-1.3895	82	1	-6.42853	8.113517	-2.6422
3	6	3.921289	-2.28118	-1.3361	83	1	-7.77801	8.427883	-0.58843
4	6	4.444023	-1.19158	-0.6572	84	6	-5.81397	4.485751	2.341403
5	6	2.64249	-4.03335	-2.9591	85	6	-7.81326	3.445102	1.189572
6	6	3.959426	-4.41608	-2.3072	86	6	-9.05451	-1.31265	-0.19308
7	1	2.072486	-4.92162	-3.2396	87	6	-8.00943	-3.0271	-1.73413
8	1	4.602149	-4.95969	-3.0025	88	1	-7.32337	-3.87535	-1.81744
9	6	5.824092	-0.86697	-0.4265	89	1	-8.99852	-3.35179	-2.07472
10	6	6.943721	-1.54576	-0.8961	90	1	-7.66323	-2.23698	-2.40925
11	6	7.964229	0.205546	0.33357	91	1	-8.72159	-0.49547	-0.842
12	6	8.141793	-0.93856	-0.4644	92	1	-10.0583	-1.61101	-0.51415
13	1	6.872824	-2.42667	-1.5174	93	1	-9.12217	-0.93267	0.830697
14	6	9.150369	0.814997	0.76225	94	1	-7.71175	2.534628	1.789976
15	6	10.28133	0.139089	0.2940	95	1	-8.49188	4.123557	1.717683
16	1	9.205107	1.701138	1.38069	96	1	-8.27362	3.177016	0.233872
17	6	11.66808	0.393641	0.47664	97	1	-4.83681	4.960805	2.212885
18	6	12.30066	1.393953	1.17848	98	1	-6.46416	5.18103	2.883167
19	6	13.78173	1.394614	1.18409	99	1	-5.6834	3.593029	2.962604
20	6	11.6031	2.412182	1.88837					
21	8	14.48211	0.575913	0.61393					
22	8	14.29804	2.419686	1.90289					
23	1	15.26502	2.341238	1.85143					
24	1	12.35742	-0.29769	-0.0046					
25	16	9.826426	-1.27327	-0.6933					
26	16	6.264925	0.539658	0.56257					
27	16	3.122663	-0.19863	-0.0585					
28	7	10.996	3.228869	2.45756					
29	8	1.819179	-3.30802	-2.0335					
30	8	4.69453	-3.23824	-1.9278					
31	1	2.819558	-3.4182	-3.8511					
32	1	3.782323	-5.03206	-1.4166					
33	6	0.469892	-0.9309	-0.5896					
34	6	0.043183	0.353901	-0.1908					
35	6	-0.53248	-1.89884	-0.8188					
36	6	-1.30054	0.65745	-0.0197					
37	1	0.774457	1.136023	-0.0077					
38	6	-1.87967	-1.59524	-0.6624					
39	1	-0.25203	-2.89694	-1.1304					
40	6	-2.29346	-0.31286	-0.2562					
41	1	-1.58807	1.654366	0.29578					
42	1	-2.62332	-2.36121	-0.8541					
43	7	-3.66173	-0.00713	-0.0898					
44	6	-4.56917	-0.99403	0.3941					
45	6	-4.23363	-1.77967	1.51201					
46	6	-5.8122	-1.17923	-0.2401					
47	6	-5.11263	-2.75075	1.99186					
48	1	-3.27753	-1.62293	2.00078					
49	6	-6.6923	-2.13619	0.24840					
50	1	-6.06352	-0.56963	-1.1031					
51	6	-6.34778	-2.9297	1.36162					
52	1	-4.83461	-3.34627	2.8570					
53	6	-8.07907	-2.50922	-0.2787					
54	6	-7.45469	-3.85195	1.63971					
55	6	-8.47427	-3.62303	0.69219					
56	6	-7.60688	-4.83109	2.62618					
57	6	-9.64626	-4.37234	0.72909					
58	6	-8.78734	-5.57974	2.65862					
59	1	-6.82443	-5.01193	3.35816					
60	6	-9.80027	-5.35362	1.71838					
61	1	-10.4393	-4.2057	0.00436					
62	1	-8.92018	-6.34346	3.41955					
63	1	-10.712	-5.94283	1.75606					
64	6	-4.15516	1.292607	-0.4059					
65	6	-3.79168	1.915297	-1.6139					
66	6	-5.01783	1.954596	0.48792					
67	6	-4.26603	3.188174	-1.9317					
68	1	-3.13341	1.393235	-2.3008					
69	6	-5.50119	3.21538	0.16279					
70	1	-5.29168	1.468022	1.41948					
71	6	-5.12635	3.840942	-1.0438					
72	1	-3.97345	3.651737	-2.8698					
73	6	-6.43559	4.113529	0.97526					
74	6	-5.77442	5.155797	-1.1104					
75	6	-6.54241	5.33376	0.05927					
76	6	-5.72737	6.152864	-2.0894					
77	6	-7.26355	6.508162	0.25205					
78	6	-6.45527	7.329913	-1.8904					
79	1	-5.13621	6.02146	-2.9916					
80	6	-7.21801	7.507972	-0.7295					

JK-201



center Number	Atomic Number	Coordinates (Angstroms)			Number	Number	X	Y	Z
		X	Y	Z	82	7	-4.47109	5.044028	0.405191
1	6	-0.36914	-1.44105	-0.32867					
2	6	-1.48093	-2.23986	-0.45742					
3	6	-2.62692	-1.39512	-0.32357					
4	1	-1.47837	-3.31102	-0.58933					
5	6	-2.1412	-0.10863	-0.13844					
6	6	1.037866	-1.69736	-0.35012					
7	6	1.679881	-2.90575	-0.55604					
8	6	3.095235	-2.8157	-0.5078					
9	6	3.572525	-1.53138	-0.28014					
10	6	1.875283	-5.10775	-1.30321					
11	6	3.192963	-5.15286	-0.54708					
12	1	1.330711	-6.04787	-1.19288					
13	1	3.854439	-5.91871	-0.95723					
14	6	4.937512	-1.1006	-0.17608					
15	6	6.083366	-1.86143	-0.38746					
16	6	7.03517	0.237925	0.166792					
17	6	7.25678	-1.10383	-0.19208					
18	1	6.046814	-2.90326	-0.67135					
19	6	8.196723	0.99676	0.35718					
20	6	9.353499	0.240019	0.144937					
21	1	8.217147	2.042373	0.634619					
22	6	10.72919	0.588589	0.224911					
23	6	11.32241	1.789494	0.54111					
24	6	12.80234	1.842452	0.540989					
25	6	10.58548	2.964311	0.86342					
26	8	13.53437	0.902742	0.281956					
27	8	13.27855	3.068223	0.865101					
28	1	14.24796	3.009587	0.840041					
29	1	11.44517	-0.20154	0.006183					
30	16	8.953535	-1.43959	-0.29777					
31	16	5.323896	0.572822	0.27424					
32	16	2.21443	-0.42076	-0.11538					
33	7	9.946574	3.904828	1.121952					
34	8	1.019288	-4.08553	-0.76677					
35	8	3.899591	-3.90539	-0.68222					
36	1	2.051406	-4.91159	-2.36884					
37	1	3.018709	-5.35311	0.517534					
38	8	-0.76581	-0.14449	-0.13249					
39	6	-4.02399	-1.87656	-0.334					
40	6	-4.92631	-1.52067	0.687412					
41	6	-4.47003	-2.74619	-1.33897					
42	6	-6.21958	-2.01757	0.691162					
43	1	-4.6226	-0.86443	1.495859					
44	6	-5.7779	-3.23891	-1.33588					
45	1	-3.79691	-3.02921	-2.14226					
46	6	-6.66901	-2.88529	-0.32048					
47	1	-6.10876	-3.90758	-2.12661					
48	6	-8.4063	-1.88384	1.597127					
49	6	-8.89703	-2.74381	0.600128					
50	1	-8.3446	-3.8334	-1.06812					
51	6	-9.26842	-1.24936	2.480644					
52	6	-10.2755	-2.9525	0.508825					
53	1	-8.8483	-0.59034	3.233339					
54	6	-10.6481	-1.47295	2.389726					
55	6	-11.1481	-2.32346	1.403607					
56	1	-10.6627	-3.61739	-0.2594					
57	1	-11.3198	-0.98121	3.085742					
58	1	-12.2157	-2.50189	1.322376					
59	6	-2.73517	1.213919	0.00671					
60	6	-2.01082	2.25919	0.60654					
61	6	-4.03126	1.491678	-0.47985					
62	6	-2.56509	3.532114	0.73141					
63	1	-1.01009	2.074715	0.979393					
64	6	-4.57697	2.754887	-0.34065					
65	1	-4.62042	0.731044	-0.97713					
66	6	-3.85753	3.798814	0.270293					
67	1	-1.9939	4.327024	1.204044					
68	6	-6.32124	4.257493	-0.92472					
69	6	-5.6345	5.325444	-0.32228					
70	1	-3.89173	5.82385	0.680239					
71	6	-7.49247	4.474873	-1.63719					
72	6	-6.14855	6.618027	-0.4534					
73	6	-8.0066	5.772383	-1.75573					
74	1	-7.99176	3.623065	-2.08725					
75	6	-7.33297	6.840825	-1.16393					
76	1	-5.62253	7.448538	0.010873					
77	1	-8.92569	5.938414	-2.30812					
78	1	-7.72101	7.85074	-1.25115					
79	8	-7.04404	-1.67103	1.748739					
80	8	-5.86824	2.953061	-0.80215					
81	7	-7.97609	-3.37709	-0.246					

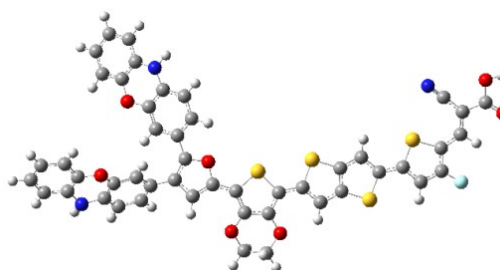
JK-POZ



center Number	Atomic Number	Coordinates (Angstroms)		
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3	6	-4.3557	-1.39054	-0.26256
4	1	-3.40708	-3.42152	-0.4574
5	6	-3.74212	-0.15172	-0.14973
6	6	-0.73949	-2.05605	-0.34686
7	6	-0.22354	-3.32934	-0.5066
8	6	1.195372	-3.37743	-0.49138
9	6	1.801109	-2.13856	-0.3359
10	6	-0.2623	-5.5737	-1.14552
11	6	1.063501	-5.71158	-0.41505
12	1	-0.89304	-6.44904	-0.97642
13	1	1.635534	-6.55926	-0.79801
14	6	3.205328	-1.84045	-0.28135
15	6	4.266791	-2.71357	-0.49292
16	6	5.431823	-0.70206	-0.03871
17	6	5.512093	-2.06399	-0.35281
18	1	4.123502	-3.75605	-0.73849
19	6	6.676958	-0.05869	0.092833
20	6	7.738975	-0.92825	-0.12036
21	1	6.808177	0.990567	0.331054
22	16	7.172768	-2.57051	-0.49007
23	16	3.766856	-0.19929	0.09977
24	16	0.562972	-0.89259	-0.19971
25	8	-1.00085	-4.4473	-0.64497
26	8	1.885197	-4.54922	-0.62983
27	1	-0.09449	-5.4483	-2.22315
28	1	0.897066	-5.84047	0.661899
29	8	-2.37673	-0.32347	-0.16869
30	6	9.144071	-0.63931	-0.07153
31	6	10.20464	-1.51405	-0.29571
32	16	9.71346	0.976061	0.306241
33	6	11.43613	-0.8699	-0.16014
34	1	10.10252	-2.56235	-0.54512
35	6	11.40306	0.485927	0.163738
36	6	12.55309	1.293358	0.339111
37	6	12.67213	2.625109	0.655003
38	6	11.55228	3.478335	0.875439
39	6	14.04058	3.183325	0.767542
40	7	10.62158	4.158164	1.051671
41	1	14.96942	4.778152	1.13434
42	8	15.0669	2.548511	0.600466
43	8	14.03996	4.500162	1.081975
44	1	13.4997	0.774795	0.201225
45	6	-5.79309	-1.73088	-0.22128
46	6	-6.34708	-2.59978	-1.17171
47	6	-6.6307	-1.23798	0.798312
48	6	-7.69654	-2.95952	-1.11769
49	1	-5.72495	-2.98704	-1.9726
50	6	-7.96596	-1.60343	0.852998
51	1	-6.24412	-0.5765	1.566067
52	6	-8.52325	-2.47038	-0.10407
53	1	-8.11086	-3.6298	-1.86664
54	6	-10.1058	-1.21062	1.795118
55	6	-10.7031	-2.0651	0.852992
56	1	-10.3019	-3.28233	-0.76948
57	6	-10.8794	-0.45245	2.662959
58	6	-12.0973	-2.14106	0.800652
59	6	-12.2762	-0.54309	2.611736
60	1	-10.3782	0.197511	3.37263
61	1	-12.5667	-2.80085	0.07506
62	6	-12.8815	-1.3867	1.680192
63	1	-12.879	0.045467	3.295639
64	1	-13.9631	-1.46273	1.629902
65	6	-4.20008	1.228626	-0.05809
66	6	-3.36532	2.223285	0.481147
67	6	-5.47158	1.610974	-0.53833
68	6	-3.78948	3.549314	0.55378
69	1	-2.38062	1.957617	0.847672
70	6	-5.88781	2.927105	-0.45103
71	1	-6.14185	0.890458	-0.99066
72	6	-5.05796	3.921353	0.099423
73	1	-3.13415	4.304518	0.980149
74	6	-7.48433	4.567036	-1.08471
75	6	-6.68489	5.588215	-0.54316
76	1	-4.88458	5.956483	0.411656
77	6	-8.63925	4.866613	-1.79401
78	6	-7.06952	6.918121	-0.7321
79	6	-9.02331	6.202013	-1.97048
80	1	-9.22809	4.048665	-2.19608
81	1	-6.45597	7.712916	-0.31511

center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	6	-8.23708	7.224479	-1.43943
83	1	-9.92999	6.432863	-2.52007
84	1	-8.52383	8.262927	-1.57183
85	7	-5.54402	5.226384	0.184549
86	7	-9.87005	-2.82621	0.021307
87	8	-8.726	-1.12583	1.907908
88	8	-7.16205	3.231166	-0.90253
89	9	12.59925	-1.52307	-0.3334

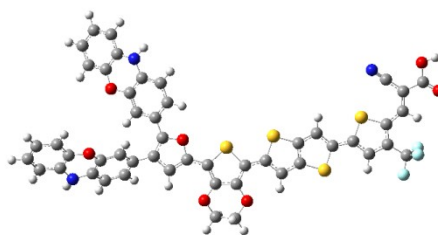
JK-POZ-1



center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.72475	-1.61886	-0.29518
2	6	-3.89758	-2.33291	-0.36633
3	6	-4.97157	-1.39449	-0.25923
4	1	-3.9811	-3.40617	-0.44316
5	6	-4.38381	-0.1429	-0.14778
6	6	-1.34251	-1.98647	-0.32491
7	6	-0.80038	-3.25003	-0.47683
8	6	0.618887	-3.26958	-0.45468
9	6	1.199095	-2.01788	-0.30198
10	6	-0.79112	-5.49717	-1.10695
11	6	0.53353	-5.60568	-0.36956
12	1	-1.40509	-6.38424	-0.93736
13	1	1.124507	-6.4429	-0.74665
14	6	2.596466	-1.69192	-0.24262
15	6	3.676156	-2.5468	-0.43748
16	6	4.798974	-0.50772	-0.00024
17	6	4.907477	-1.87169	-0.29771
18	1	3.554613	-3.59471	-0.67127
19	6	6.030691	0.160621	0.131711
20	6	7.110534	-0.69114	-0.06433
21	1	6.140371	1.214837	0.358766
22	16	6.578175	-2.34823	-0.41842
23	16	3.123882	-0.03552	0.121851
24	16	-0.06447	-0.79643	-0.1763
25	8	-1.55449	-4.3837	-0.61441
26	8	1.332718	-4.42759	-0.58452
27	1	-0.62071	-5.37257	-2.18424
28	1	0.364557	-5.73397	0.707038
29	8	-3.01519	-0.28682	-0.16021
30	6	8.509681	-0.37535	-0.00987
31	6	9.590613	-1.23215	-0.21108
32	16	9.061396	1.243161	0.342039
33	6	10.83256	-0.59414	-0.08386
34	1	9.483925	-2.28385	-0.44247
35	6	10.7522	0.773659	0.219202
36	6	11.85615	1.654243	0.401665
37	6	11.89107	2.99416	0.697647
38	6	10.72976	3.797598	0.888304
39	6	13.22878	3.629742	0.823439
40	7	9.771828	4.443984	1.041957
41	1	14.05964	5.280448	1.1796
42	8	14.2882	3.047654	0.682799
43	8	13.14885	4.947826	1.116113
44	1	12.84	1.206102	0.291669
45	6	-6.40191	-1.76411	-0.2235
46	6	-6.9342	-2.64436	-1.17585
47	6	-7.25336	-1.2882	0.792688
48	6	-8.27623	-3.03158	-1.12703
49	1	-6.30112	-3.019	-1.97416
50	6	-8.58107	-1.68089	0.842285
51	1	-6.88341	-0.61874	1.561735
52	6	-9.11674	-2.55925	-0.11678
53	1	-8.67382	-3.71033	-1.87741
54	6	-10.7322	-1.33205	1.77614
55	6	-11.3081	-2.19873	0.831908
56	1	-10.8757	-3.40795	-0.78867
57	6	-11.5245	-0.59007	2.641061
58	6	-12.7002	-2.30354	0.774367
59	6	-12.9189	-0.7096	2.584642
60	1	-11.0395	0.070099	3.352571
61	1	-13.1531	-2.97292	0.04711
62	6	-13.5031	-1.56555	1.650921
63	1	-13.5363	-0.13367	3.266268
64	1	-14.5827	-1.66396	1.596628
65	6	-4.87035	1.227917	-0.06245
66	6	-4.05703	2.241921	0.473601
67	6	-6.14912	1.581809	-0.54533
68	6	-4.50883	3.55904	0.540677
69	1	-3.06739	1.998338	0.842142
70	6	-6.59281	2.889255	-0.46359
71	1	-6.80386	0.845742	-0.99531
72	6	-5.78439	3.902795	0.083721
73	1	-3.86985	4.329402	0.964716
74	6	-8.22381	4.492856	-1.10296
75	6	-7.44634	5.532582	-0.56477
76	1	-5.65422	5.942286	0.389081
77	6	-9.3853	4.765419	-1.8124
78	6	-7.85964	6.853338	-0.75722
79	6	-9.79813	6.091721	-1.99246
80	1	-9.95659	3.933827	-2.21179
81	1	-7.26319	7.662361	-0.34281

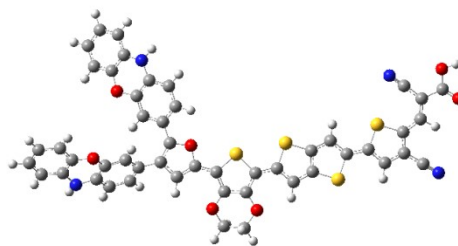
center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	6	-9.03387	7.132424	-1.46479
83	1	-10.7099	6.301389	-2.54218
84	1	-9.34302	8.164059	-1.59998
85	7	-6.29752	5.197564	0.163248
86	7	-10.4564	-2.94243	0.003374
87	8	-9.35479	-1.21867	1.894018
88	8	-7.87262	3.164736	-0.91745
89	6	12.13058	-1.3342	-0.26189
90	9	12.87869	-0.82104	-1.27183
91	9	12.90284	-1.28993	0.853798
92	9	11.92232	-2.64073	-0.5477

JK-POZ-2



center Number	Atomic Number	Coordinates (Angstroms)			center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	-2.22232	-1.64976	-0.30471	81	1	-6.62661	7.695656	-0.32508
2	6	-3.4056	-2.34667	-0.37416	82	6	-8.40578	7.193675	-1.44649
3	6	-4.46556	-1.39319	-0.26243	83	1	-10.0945	6.389193	-2.52416
4	1	-3.50478	-3.41846	-0.45288	84	1	-8.7003	8.229922	-1.579
5	6	-3.85937	-0.15035	-0.15005	85	7	-5.69566	5.216082	0.174046
6	6	-0.84583	-2.03731	-0.3392	86	7	-9.97142	-2.86149	0.013584
7	6	-0.32267	-3.30833	-0.49668	87	8	-8.83983	-1.15539	1.902604
8	6	1.096061	-3.34864	-0.47903	88	8	-7.30085	3.20853	-0.90939
9	6	1.694916	-2.10577	-0.3242	89	6	12.58462	-1.50904	-0.30836
10	6	-0.34818	-5.55266	-1.13566	90	7	13.58176	-2.09188	-0.45404
11	6	0.97693	-5.68379	-0.40281					
12	1	-0.9745	-6.4314	-0.96798					
13	1	1.554754	-6.52755	-0.7856					
14	6	3.096787	-1.80066	-0.26807					
15	6	4.163316	-2.67085	-0.46918					
16	6	5.316985	-0.64967	-0.02876					
17	6	5.404527	-2.01424	-0.33113					
18	1	4.025653	-3.71606	-0.70605					
19	6	6.558741	-0.00017	0.101298					
20	6	7.625109	-0.86724	-0.10114					
21	1	6.684229	1.051689	0.331185					
22	16	7.067581	-2.515	-0.45884					
23	16	3.649426	-0.15336	0.100109					
24	16	0.449641	-0.86639	-0.19067					
25	8	-1.09364	-4.43029	-0.6358					
26	8	1.792569	-4.51616	-0.61461					
27	1	-0.17936	-5.42577	-2.21292					
28	1	0.80947	-5.81456	0.673675					
29	8	-2.49308	-0.3139	-0.16624					
30	6	9.028975	-0.57177	-0.05027					
31	6	10.09625	-1.43843	-0.26157					
32	16	9.600302	1.043354	0.31308					
33	6	11.35179	-0.81065	-0.13322					
34	1	9.982803	-2.48835	-0.50113					
35	6	11.28176	0.559792	0.181198					
36	6	12.4115	1.404203	0.360434					
37	6	12.48638	2.740015	0.665208					
38	6	11.34388	3.566921	0.868716					
39	6	13.84055	3.341802	0.78608					
40	7	10.3975	4.227818	1.031801					
41	1	14.71259	4.970282	1.148123					
42	8	14.88291	2.733694	0.633821					
43	8	13.79392	4.659087	1.088305					
44	1	13.37716	0.916573	0.236857					
45	6	-5.901	-1.74201	-0.22329					
46	6	-6.44855	-2.61363	-1.17492					
47	6	-6.74272	-1.25457	0.795552					
48	6	-7.79592	-2.98135	-1.12277					
49	1	-5.82319	-2.99676	-1.97528					
50	6	-8.07585	-1.62796	0.848456					
51	1	-6.36105	-0.59121	1.56416					
52	6	-8.62679	-2.49771	-0.10987					
53	1	-8.20533	-3.65362	-1.87262					
54	6	-10.2191	-1.24941	1.788948					
55	6	-10.81	-2.10692	0.845657					
56	1	-10.3996	-3.32081	-0.77731					
57	6	-10.9982	-0.49734	2.657118					
58	6	-12.2036	-2.19224	0.792398					
59	6	-12.3943	-0.59728	2.604942					
60	1	-10.5018	0.155194	3.367811					
61	1	-12.6682	-2.85445	0.065902					
62	6	-12.9934	-1.444	1.672208					
63	1	-13.0014	-0.0135	3.289094					
64	1	-14.0744	-1.52725	1.621227					
65	6	-4.32605	1.227049	-0.06106					
66	6	-3.49771	2.228081	0.47635					
67	6	-5.6001	1.600211	-0.54196					
68	6	-3.93047	3.551381	0.546643					
69	1	-2.51137	1.969491	0.843528					
70	6	-6.02485	2.913713	-0.45725					
71	1	-6.26575	0.874504	-0.99278					
72	6	-5.20137	3.914399	0.091478					
73	1	-3.28017	4.311601	0.971756					
74	6	-7.63323	4.541995	-1.09158					
75	6	-6.84047	5.569233	-0.55182					
76	1	-5.04195	5.951047	0.401895					
77	6	-8.79138	4.832734	-1.79924					
78	6	-7.23498	6.896207	-0.74074					
79	6	-9.18533	6.165224	-1.97583					
80	1	-9.37491	4.010341	-2.19996					

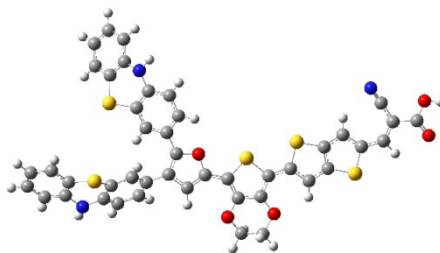
JK-POZ-3



center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.11906	-1.5388	-0.2951
2	6	-1.22619	-2.34233	-0.43361
3	6	-2.37654	-1.51081	-0.25825
4	1	-1.21715	-3.4088	-0.59916
5	6	-1.89856	-0.22735	-0.04002
6	6	1.289848	-1.78254	-0.34367
7	6	1.938194	-2.97849	-0.59576
8	6	3.353607	-2.87811	-0.56426
9	6	3.823481	-1.59766	-0.30309
10	6	2.140795	-5.15542	-1.41216
11	6	3.469252	-5.21199	-0.67598
12	1	1.605146	-6.10279	-1.32225
13	1	4.130913	-5.95969	-1.11803
14	6	5.186579	-1.15874	-0.20357
15	6	6.335075	-1.90146	-0.45885
16	6	7.277738	0.184632	0.157339
17	6	7.505181	-1.14112	-0.25303
18	1	6.302894	-2.93262	-0.77986
19	6	8.435821	0.946406	0.358288
20	6	9.595252	0.20796	0.101945
21	1	8.451675	1.981461	0.67308
22	6	10.96936	0.56549	0.174543
23	6	11.55699	1.759142	0.525626
24	6	13.03653	1.825258	0.506042
25	6	10.81508	2.914907	0.901235
26	8	13.7722	0.901948	0.202598
27	8	13.50693	3.042462	0.868056
28	1	14.47637	2.993773	0.827229
29	1	11.6885	-0.20988	-0.08318
30	16	9.202859	-1.45795	-0.39523
31	16	5.565674	0.500405	0.301835
32	16	2.459321	-0.50401	-0.08564
33	7	10.17219	3.839641	1.203056
34	8	1.284206	-4.15649	-0.83385
35	8	4.16393	-3.95509	-0.78362
36	1	2.300259	-4.92627	-2.47378
37	1	3.311747	-5.44532	0.384493
38	8	-0.52308	-0.25221	-0.05352
39	6	-3.77119	-2.00031	-0.26413
40	6	-4.65607	-1.69872	0.785921
41	6	-4.23519	-2.8242	-1.30102
42	6	-5.95286	-2.20921	0.80944
43	1	-4.31931	-1.07516	1.608413
44	6	-5.54329	-3.30713	-1.30317
45	1	-3.57659	-3.06655	-2.12962
46	6	-6.41731	-3.01284	-0.24905
47	1	-5.89174	-3.92051	-2.13082
48	6	-8.59122	-1.99273	1.457813
49	6	-8.79807	-2.81194	0.333406
50	1	-7.97028	-4.0612	-1.0522
51	6	-9.65931	-1.2808	2.008743
52	6	-10.0872	-2.92008	-0.20497
53	1	-9.48038	-0.63359	2.862234
54	6	-10.9471	-1.41144	1.481263
55	6	-11.1579	-2.23827	0.375899
56	1	-10.2489	-3.54697	-1.0789
57	1	-11.7726	-0.86729	1.928619
58	1	-12.1521	-2.34511	-0.04718
59	6	-2.50084	1.086178	0.153847
60	6	-1.777	2.117391	0.781568
61	6	-3.79936	1.375079	-0.31084
62	6	-2.33158	3.383162	0.938168
63	1	-0.77107	1.927318	1.138065
64	6	-4.3719	2.628511	-0.1141
65	1	-4.37193	0.613424	-0.82743
66	6	-3.63646	3.657459	0.504872
67	1	-1.74988	4.170812	1.411034
68	6	-6.02828	4.650446	-0.90305
69	6	-5.13064	5.479146	-0.20591
70	1	-3.58408	5.598818	1.122139
71	6	-6.93857	5.210629	-1.80248
72	6	-5.18018	6.864696	-0.41007
73	6	-6.99806	6.59519	-1.9847
74	1	-7.61225	4.557538	-2.34945
75	6	-6.11897	7.420615	-1.28062
76	1	-4.48215	7.506746	0.122181
77	1	-7.72182	7.019772	-2.67295
78	1	-6.15052	8.497407	-1.41558
79	7	-7.72443	-3.52077	-0.23371
80	7	-4.20198	4.924424	0.691153
81	16	-6.08022	2.899164	-0.55757

center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	16	-6.98686	-1.94712	2.241285

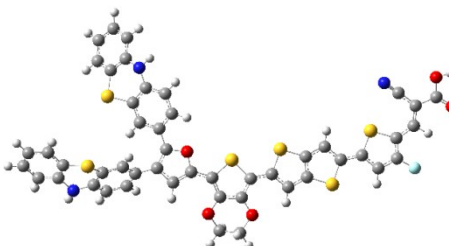
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center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.84088	-1.76655	-0.27534
2	6	-3.02311	-2.46345	-0.35702
3	6	-4.08366	-1.51643	-0.199
4	1	-3.12096	-3.53188	-0.47407
5	6	-3.47943	-0.27781	-0.04816
6	6	-0.46331	-2.14901	-0.33962
7	6	0.060516	-3.41189	-0.54758
8	6	1.480058	-3.44912	-0.54788
9	6	2.077539	-2.21148	-0.35635
10	6	0.032678	-5.63415	-1.26097
11	6	1.366739	-5.78542	-0.5485
12	1	-0.58978	-6.51942	-1.11448
13	1	1.941315	-6.61538	-0.96495
14	6	3.480204	-1.90404	-0.3057
15	6	4.545709	-2.761	-0.5578
16	6	5.700257	-0.75712	-0.04697
17	6	5.787608	-2.10673	-0.40824
18	1	4.407771	-3.79559	-0.83744
19	6	6.941962	-0.10869	0.093811
20	6	8.007968	-0.96214	-0.15981
21	1	7.067758	0.932792	0.366539
22	16	7.45048	-2.59512	-0.57974
23	16	4.033169	-0.27256	0.125672
24	16	0.831541	-0.98082	-0.1658
25	8	-0.70945	-4.53044	-0.7165
26	8	2.177249	-4.61001	-0.73292
27	1	0.188536	-5.47208	-2.33547
28	1	1.212298	-5.95109	0.525191
29	8	-2.11301	-0.43736	-0.08543
30	6	9.411557	-0.66398	-0.11551
31	6	10.47612	-1.52278	-0.37815
32	16	9.972523	0.942705	0.30837
33	6	11.70421	-0.87374	-0.23392
34	1	10.37937	-2.56334	-0.66005
35	6	11.66409	0.470582	0.133809
36	6	12.80993	1.280979	0.323911
37	6	12.92192	2.602677	0.681222
38	6	11.79779	3.439472	0.93969
39	6	14.28728	3.16794	0.798438
40	7	10.86362	4.105766	1.146549
41	1	15.20726	4.757764	1.207175
42	8	15.31653	2.546825	0.601126
43	8	14.27956	4.473905	1.154832
44	1	13.75898	0.774518	0.160247
45	6	-5.51884	-1.86761	-0.15742
46	6	-6.08324	-2.6862	-1.1477
47	6	-6.34665	-1.43726	0.894292
48	6	-7.43129	-3.04003	-1.10397
49	1	-5.46979	-3.02635	-1.97657
50	6	-7.6855	-1.8187	0.964792
51	1	-5.9329	-0.81483	1.68177
52	6	-8.24872	-2.61821	-0.0478
53	1	-7.85574	-3.65162	-1.89674
54	6	-10.2757	-1.32322	1.653614
55	6	-10.5856	-2.16547	0.570626
56	1	-9.91267	-3.54514	-0.77442
57	6	-11.2585	-0.49021	2.193461
58	6	-11.8915	-2.17243	0.062729
59	6	-12.565	-0.51934	1.697493
60	1	-10.9991	0.172086	3.01408
61	1	-12.1323	-2.81711	-0.77948
62	6	-12.879	-1.36782	0.633803
63	1	-13.3247	0.119354	2.136527
64	1	-13.8885	-1.39689	0.235265
65	6	-3.94783	1.095481	0.095862
66	6	-3.11591	2.077684	0.665451
67	6	-5.22113	1.48896	-0.36158
68	6	-3.54282	3.397065	0.773432
69	1	-2.1262	1.806183	1.014636
70	6	-5.66627	2.799473	-0.21258
71	1	-5.87428	0.764952	-0.83491
72	6	-4.82335	3.777806	0.348381
73	1	-2.87881	4.144249	1.201502
74	6	-7.13292	4.936879	-1.0693
75	6	-6.14657	5.703726	-0.42302
76	1	-4.5727	5.729823	0.877493
77	6	-8.00032	5.543143	-1.98119
78	6	-6.06467	7.077027	-0.68999
79	6	-7.92807	6.91741	-2.22595
80	1	-8.74397	4.935546	-2.48849
81	1	-5.29808	7.670559	-0.1972

center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	6	-6.96034	7.683111	-1.57244
83	1	-8.61926	7.379958	-2.92317
84	1	-6.88938	8.750755	-1.75631
85	7	-5.26099	5.100805	0.486408
86	7	-9.59768	-2.99703	0.014722
87	9	12.87031	-1.51193	-0.43942
88	16	-7.34841	3.21609	-0.6433
89	16	-8.65633	-1.39811	2.403127

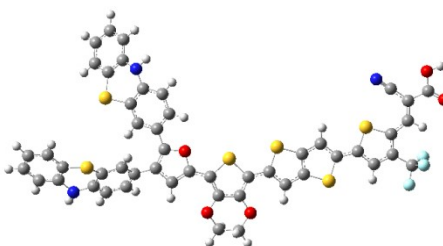
JK-PTZ-1



center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-2.44265	-1.72309	-0.25218
2	6	-3.61038	-2.44388	-0.33675
3	6	-4.69038	-1.51762	-0.18922
4	1	-3.68626	-3.5146	-0.44908
5	6	-4.11179	-0.26632	-0.0413
6	6	-1.05764	-2.07838	-0.30704
7	6	-0.50789	-3.33195	-0.50545
8	6	0.911877	-3.34112	-0.49815
9	6	1.483904	-2.09065	-0.3103
10	6	-0.48809	-5.55784	-1.20765
11	6	0.844818	-5.67927	-0.48741
12	1	-1.09378	-6.45443	-1.05991
13	1	1.438098	-6.49944	-0.89691
14	6	2.879634	-1.75572	-0.25435
15	6	3.963132	-2.59423	-0.49267
16	6	5.075566	-0.56382	0.006643
17	6	5.191027	-1.91488	-0.34205
18	1	3.84682	-3.63374	-0.76369
19	6	6.303791	0.109212	0.149002
20	6	7.387439	-0.72613	-0.09068
21	1	6.408106	1.155232	0.413384
22	16	6.863719	-2.3732	-0.49945
23	16	3.398578	-0.10986	0.165235
24	16	0.212812	-0.88384	-0.13249
25	8	-1.25474	-4.46618	-0.67262
26	8	1.632844	-4.48867	-0.67301
27	1	-0.32982	-5.39799	-2.2821
28	1	0.688064	-5.84292	0.586219
29	8	-2.74232	-0.39867	-0.07035
30	6	8.784983	-0.40132	-0.04082
31	6	9.869767	-1.24119	-0.28663
32	16	9.32833	1.207248	0.364916
33	6	11.10833	-0.59823	-0.15023
34	1	9.768404	-2.28433	-0.55605
35	6	11.02093	0.756462	0.204787
36	6	12.12032	1.63874	0.407229
37	6	12.14826	2.966716	0.752801
38	6	10.98302	3.752809	0.987027
39	6	13.48254	3.608289	0.886693
40	7	10.0219	4.384918	1.175975
41	1	14.30438	5.251544	1.294752
42	8	14.54455	3.040475	0.711934
43	8	13.39563	4.913693	1.229415
44	1	13.10622	1.20312	0.268927
45	6	-6.11845	-1.89736	-0.1539
46	6	-6.66106	-2.73034	-1.14434
47	6	-6.9602	-1.48033	0.892103
48	6	-8.00193	-3.11104	-1.10639
49	1	-6.03658	-3.06082	-1.96888
50	6	-8.29144	-1.88842	0.957019
51	1	-6.56318	-0.84709	1.679597
52	6	-8.8332	-2.70233	-0.05586
53	1	-8.40983	-3.73362	-1.89928
54	6	-10.8946	-1.44348	1.631358
55	6	-11.1819	-2.29511	0.549488
56	1	-10.4744	-3.66481	-0.78805
57	6	-11.8969	-0.62909	2.163816
58	6	-12.4849	-2.33024	0.03524
59	6	-13.2	-0.68633	1.661543
60	1	-11.6551	0.040822	2.983648
61	1	-12.7082	-2.98223	-0.80613
62	6	-13.4914	-1.54423	0.598974
63	1	-13.9747	-0.06197	2.094904
64	1	-14.4981	-1.59512	0.195594
65	6	-4.60837	1.09789	0.093401
66	6	-3.79843	2.099965	0.660093
67	6	-5.88798	1.462865	-0.37019
68	6	-4.25238	3.410945	0.759321
69	1	-2.80458	1.850616	1.013992
70	6	-6.36011	2.764829	-0.22998
71	1	-6.52483	0.723107	-0.84135
72	6	-5.539	3.763246	0.328063
73	1	-3.6051	4.173823	1.185324
74	6	-7.86763	4.867033	-1.10259
75	6	-6.89903	5.657419	-0.45787
76	1	-5.32973	5.722855	0.846892
77	6	-8.74467	5.450454	-2.02014
78	6	-6.84448	7.03063	-0.73211
79	6	-8.69985	6.824567	-2.27223
80	1	-9.47433	4.825056	-2.52613
81	1	-6.09159	7.642398	-0.24049

center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	6	-7.74984	7.613457	-1.62031
83	1	-9.39839	7.269057	-2.97384
84	1	-7.70022	8.681319	-1.80981
85	7	-6.00374	5.077727	0.457173
86	7	-10.1745	-3.10794	0.000854
87	6	12.40987	-1.32045	-0.37098
88	9	13.14235	-0.76292	-1.36875
89	9	13.1944	-1.31261	0.736911
90	9	12.20823	-2.61667	-0.70433
91	16	-9.27782	-1.48312	2.389099
92	16	-8.04912	3.144565	-0.66769

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center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.94712	-1.75544	-0.26789
2	6	-3.12532	-2.4593	-0.35098
3	6	-4.19147	-1.51845	-0.19666
4	1	-3.21676	-3.52845	-0.46674
5	6	-3.59455	-0.27592	-0.0464
6	6	-0.56769	-2.13027	-0.32877
7	6	-0.03674	-3.39097	-0.53414
8	6	1.382608	-3.42056	-0.5319
9	6	1.973212	-2.17896	-0.3412
10	6	-0.0515	-5.61328	-1.24714
11	6	1.281937	-5.75777	-0.53221
12	1	-0.66952	-6.50181	-1.10192
13	1	1.862183	-6.58388	-0.94834
14	6	3.373548	-1.86461	-0.28895
15	6	4.444111	-2.7188	-0.53138
16	6	5.587214	-0.7051	-0.03328
17	6	5.68191	-2.05748	-0.38373
18	1	4.311836	-3.75622	-0.80298
19	6	6.825525	-0.05051	0.106065
20	6	7.895892	-0.9016	-0.13767
21	1	6.945535	0.993699	0.371055
22	16	7.347174	-2.54025	-0.54642
23	16	3.91753	-0.22685	0.130524
24	16	0.720176	-0.95474	-0.15375
25	8	-0.80041	-4.51348	-0.70357
26	8	2.086412	-4.57731	-0.71375
27	1	0.105226	-5.44998	-2.32128
28	1	1.126631	-5.92509	0.541023
29	8	-2.22728	-0.42751	-0.08045
30	6	9.298273	-0.59697	-0.09161
31	6	10.36954	-1.44765	-0.34265
32	16	9.861089	1.009641	0.319161
33	6	11.62173	-0.81447	-0.20654
34	1	10.26156	-2.48995	-0.61566
35	6	11.54448	0.544037	0.153926
36	6	12.66982	1.391114	0.349486
37	6	12.73759	2.716471	0.697646
38	6	11.59091	3.526938	0.94021
39	6	14.08846	3.324902	0.824542
40	7	10.6411	4.174241	1.134782
41	1	14.95139	4.947685	1.231517
42	8	15.13363	2.730412	0.641417
43	8	14.03469	4.630913	1.170767
44	1	13.63779	0.915531	0.199795
45	6	-5.62471	-1.87781	-0.15758
46	6	-6.18263	-2.69973	-1.14876
47	6	-6.45671	-1.45203	0.892672
48	6	-7.5287	-3.06123	-1.10728
49	1	-5.56588	-3.03648	-1.97657
50	6	-7.79345	-1.84115	0.961021
51	1	-6.04791	-0.82714	1.680803
52	6	-8.35036	-2.64397	-0.05253
53	1	-7.94826	-3.67534	-1.90067
54	6	-10.3876	-1.36134	1.6462
55	6	-10.6908	-2.20522	0.56265
56	1	-10.0077	-3.58065	-0.78177
57	6	-11.3762	-0.53455	2.184969
58	6	-11.996	-2.22015	0.052997
59	6	-12.6818	-0.57162	1.687228
60	1	-11.122	0.129098	3.006132
61	1	-12.2316	-2.86613	-0.78965
62	6	-12.9892	-1.42177	0.622931
63	1	-13.446	0.062213	2.125431
64	1	-13.9979	-1.45701	0.223072
65	6	-4.07153	1.094585	0.094493
66	6	-3.24639	2.083041	0.663178
67	6	-5.34684	1.479124	-0.36509
68	6	-3.6817	3.399848	0.768186
69	1	-2.25546	1.818419	1.014182
70	6	-5.80038	2.787042	-0.21924
71	1	-5.99497	0.750063	-0.83755
72	6	-4.96412	3.771783	0.340776
73	1	-3.02301	4.151997	1.195753
74	6	-7.28048	4.913408	-1.08031
75	6	-6.29953	5.687724	-0.43484
76	1	-4.72635	5.726278	0.866481
77	6	-8.15155	5.512556	-1.99341
78	6	-6.22658	7.061125	-0.70371
79	6	-8.08825	6.886898	-2.24015
80	1	-8.891	4.899343	-2.50007
81	1	-5.46416	7.660444	-0.21146

center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
82	6	-7.12588	7.659966	-1.5874
83	1	-8.78223	7.343843	-2.93827
84	1	-7.06197	8.727783	-1.77279
85	7	-5.40998	5.092055	0.475646
86	7	-9.69705	-3.03047	0.007662
87	6	12.85789	-1.49686	-0.41752
88	7	13.85783	-2.06659	-0.59281
89	16	-7.48482	3.191854	-0.6519
90	16	-8.76877	-1.42637	2.397923

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