

**Dataset: Experimentally Estimated Energy Levels (HOMO(D) and LUMO(D) of Donors, HOMO(A) and LUMO(A) of Acceptors, and HOMO(T) and LUMO(T) of the Third Components) and the Device performance at different doping ratios (T(%), Voc, Jsc, FF, and PCE)**

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.18	-3.77	-6	-4	-5.15	-3.1	20	0.82	17.78	76.5	11.01	1
-5.18	-3.77	-6	-4	-5.15	-3.1	0	0.8	16.35	71.1	9.1	□
-5.18	-3.77	-6	-4	-5.15	-3.1	10	0.81	17.16	73.3	10.03	□
-5.18	-3.77	-6	-4	-5.15	-3.1	30	0.83	17.41	71.6	10.16	□
-5.1	-3.4	-5.8	-4.2	-5.91	-4.1	0	0.87	15.2	64	8.4	2
-5.1	-3.4	-5.8	-4.2	-5.91	-4.1	28	0.87	16.3	72	10.4	□
-5.1	-3.4	-5.91	-4.1	-5.8	-4.2	33	0.81	14.1	60	6.9	2
-5.1	-3.4	-5.91	-4.1	-5.8	-4.2	0	0.88	13.2	72	8.2	□
-5.36	-3.02	-5.61	-3.76	-6.08	-4.1	0	1.05	14.57	58	8.92	3
-5.36	-3.02	-5.61	-3.76	-6.08	-4.1	33	0.94	16.12	63	9.62	□
-5.36	-3.02	-5.61	-3.76	-6.08	-4.1	100	0.93	10.41	57	5.59	□
-5.16	-2.93	-5.61	-3.76	-6.08	-4.1	0	0.88	15.19	61	8.22	3
-5.16	-2.93	-5.61	-3.76	-6.08	-4.1	33	0.83	16.82	65	9.16	□
-5.16	-2.93	-5.61	-3.76	-6.08	-4.1	100	0.79	12.85	62	6.35	□
-5.15	-3.55	-6.09	-3.9	-5.52	-3.51	0	0.77	17.02	60.8	8	4
-5.15	-3.55	-6.09	-3.9	-5.52	-3.51	5	0.77	17.24	61.6	8.2	□
-5.15	-3.55	-6.09	-3.9	-5.52	-3.51	10	0.77	17.54	63.3	8.5	□
-5.15	-3.55	-6.09	-3.9	-5.52	-3.51	15	0.768	19.15	64.2	9.4	□
-5.15	-3.55	-6.09	-3.9	-5.52	-3.51	20	0.77	17.34	62	8.3	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.33	-2.92	-5.43	-3.8	-5.96	-3.98	0	0.87	18.42	62.3	9.93	5
-5.33	-2.92	-5.43	-3.8	-5.96	-3.98	17	0.86	20.5	63.6	11.16	□
-5.33	-2.92	-5.43	-3.8	-5.96	-3.98	33	0.86	20.61	63.4	11.17	□
-5.33	-2.92	-5.43	-3.8	-5.96	-3.98	50	0.88	20.84	66.7	12.07	□
-5.33	-2.92	-5.96	-3.98	-5.43	-3.8	0	0.83	13.33	69.08	7.63	5
-5.33	-2.92	-5.96	-3.98	-5.43	-3.8	17	0.85	17.96	68	10.35	□
-5.33	-2.92	-5.96	-3.98	-5.43	-3.8	33	0.87	19.57	67	11.35	□
-5.3	-2.9	-5.5	-3.8	-6	-4	0	0.902	15.06	69	9.38	6
-5.3	-2.9	-5.5	-3.8	-6	-4	20	0.892	15.98	71.7	10.22	□
-5.3	-2.9	-5.5	-3.8	-6	-4	100	0.856	13.64	70.3	8.21	□
-5.47	-3.83	-6.07	-4.03	-5.64	-3.98	0	0.76	5.87	53.8	2.4	7
-5.47	-3.83	-6.07	-4.03	-5.64	-3.98	25	0.76	17.54	65.5	8.72	□
-5.47	-3.83	-6.07	-4.03	-5.64	-3.98	37.5	0.75	21.12	63.9	10.17	□
-5.47	-3.83	-6.07	-4.03	-5.64	-3.98	50	0.76	19.76	64.3	9.53	□
-5.47	-3.83	-5.64	-3.98	-6.07	-4.03	0	0.79	13.56	65.1	6.97	7
-5.47	-3.83	-5.64	-3.98	-6.07	-4.03	25	0.77	17.59	66.3	8.98	□
-5.47	-3.83	-5.64	-3.98	-6.07	-4.03	37.5	0.77	17.8	68.2	9.27	□
-5.51	-3.62	-5.66	-4.09	-6	-4	0	0.838	26.19	75.84	16.65	8
-5.51	-3.62	-5.66	-4.09	-6	-4	8	0.847	26.44	77.65	17.39	□
-5.51	-3.62	-5.66	-4.09	-6	-4	50	0.847	23.47	73.18	14.56	□
-5.51	-3.62	-5.66	-4.09	-6	-4	100	0.911	12.5	73.22	8.34	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.54	-3.65	-5.65	-4.1	-5.87	-3.91	0	0.83	25.12	74.53	15.56	9
-5.54	-3.65	-5.65	-4.1	-5.87	-3.91	8	0.837	26.12	76.5	16.72	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	0	0.79	14.75	70	8.16	10
-5.45	-3.69	-6	-4.1	-5.52	-3.87	10	0.82	15.5	71	9.02	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	20	0.84	14.88	69	8.62	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	40	0.88	13.68	60	7.22	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	60	0.91	10.23	42	3.91	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	80	0.98	7.71	39	2.95	□
-5.45	-3.69	-6	-4.1	-5.52	-3.87	100	1.11	8.4	55	5.16	□
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	0	0.75	15.51	68.53	7.97	11
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	5	0.74	16.47	68.99	8.41	□
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	10	0.74	16.48	70.75	8.63	□
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	15	0.74	17.55	70.92	9.21	□
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	30	0.74	15.94	65.55	7.73	□
-5.51	-3.31	-5.9	-3.86	-5.23	-3.78	50	0.73	15.13	62.64	6.92	□
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	0	0.75	15.51	68.53	7.97	11
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	5	0.75	16.57	70.68	8.78	□
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	10	0.74	17.04	70.17	8.85	□
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	15	0.75	15.99	69.77	8.26	□
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	30	0.76	15.17	69.76	8.04	□
-5.51	-3.31	-5.9	-3.86	-5.14	-3.52	50	0.76	14.21	62.71	6.77	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.24	-3.62	-6.1	-3.9	-5.54	-2.8	0	0.78	17.72	65.29	8.98	12
-5.24	-3.62	-6.1	-3.9	-5.54	-2.8	5	0.78	18.02	67.51	9.59	□
-5.24	-3.62	-6.1	-3.9	-5.54	-2.8	10	0.79	20.01	68.07	10.56	□
-5.24	-3.62	-6.1	-3.9	-5.54	-2.8	15	0.79	18.53	66.71	9.62	□
-5.24	-3.62	-6.1	-3.9	-5.54	-2.8	20	0.79	17.51	66.69	9.06	□
-5.15	-3.31	-6.1	-3.9	-5.54	-2.8	0	0.72	16.09	68.01	7.92	12
-5.15	-3.31	-6.1	-3.9	-5.54	-2.8	5	0.72	16.67	71.22	8.59	□
-5.15	-3.31	-6.1	-3.9	-5.54	-2.8	10	0.73	17.7	72.64	9.42	□
-5.15	-3.31	-6.1	-3.9	-5.54	-2.8	15	0.73	15.94	71.55	8.37	□
-5.15	-3.31	-6.1	-3.9	-5.54	-2.8	20	0.73	15.4	69.31	7.84	□
-5.39	-3.12	-5.5	-3.88	-5.55	-3.67	0	0.701	22.32	60	9.39	13
-5.39	-3.12	-5.5	-3.88	-5.55	-3.67	30	0.711	25.13	68	12.06	□
-5.39	-3.12	-5.5	-3.88	-5.55	-3.67	100	0.819	15.26	62	7.74	□
-5.45	-3.26	-5.15	-4.1	-5.96	-4	0	0.849	22.43	55.82	10.58	14
-5.45	-3.26	-5.15	-4.1	-5.96	-4	17	0.86	24.64	62.04	13.15	□
-5.45	-3.26	-5.15	-4.1	-5.96	-4	100	0.913	12.16	59.55	6.58	□
-5.54	-2.98	-5.65	-4.1	-6	-4	0	0.851	24.64	71.67	15.03	15
-5.54	-2.98	-5.65	-4.1	-6	-4	14	0.85	25.32	74.69	16.07	□
-5.54	-2.98	-5.65	-4.1	-6	-4	25	0.847	25.12	71	15.11	□
-5.54	-2.98	-5.65	-4.1	-6	-4	100	0.94	8.32	55.12	4.31	□
-5.24	-3.62	-6.1	-3.7	-5.13	-2.8	0	0.78	18.26	65.49	9.26	16

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.24	-3.62	-6.1	-3.7	-5.13	-2.8	5	0.78	18.61	69.74	10.08	□
-5.24	-3.62	-6.1	-3.7	-5.13	-2.8	10	0.78	22.26	70.71	12.23	□
-5.24	-3.62	-6.1	-3.7	-5.13	-2.8	15	0.77	20.88	70.29	11.25	□
-5.24	-3.62	-6.1	-3.7	-5.13	-2.8	20	0.76	18.93	66.63	9.81	□
-5.25	-3.2	-6	-4	-5.38	-2.83	0	0.79	18.2	71.4	10.31	17
-5.25	-3.2	-6	-4	-5.38	-2.83	5	0.78	18.3	73.7	10.6	□
-5.25	-3.2	-6	-4	-5.38	-2.83	10	0.78	18.6	75.7	11	□
-5.25	-3.2	-6	-4	-5.38	-2.83	15	0.78	18.5	74.8	10.86	□
-5.25	-3.2	-6	-4	-5.38	-2.83	20	0.77	18.4	73.9	10.59	□
-5.23	-3.65	-6	-4.1	-5.21	-3.41	0	0.795	16.51	63.06	8.28	18
-5.23	-3.65	-6	-4.1	-5.21	-3.41	5	0.795	16.92	64	8.62	□
-5.23	-3.65	-6	-4.1	-5.21	-3.41	10	0.801	17.36	65.21	9.11	□
-5.23	-3.65	-6	-4.1	-5.21	-3.41	15	0.806	17.6	65.62	9.3	□
-5.23	-3.65	-6	-4.1	-5.21	-3.41	20	0.79	16.83	66.23	8.83	□
-5.23	-3.65	-6	-4.1	-5.21	-3.41	25	0.795	16.31	62.11	7.92	□
-5.32	-3.48	-5.65	-4.1	-5.96	-4	0	0.79	22.86	69.37	12.55	19
-5.32	-3.48	-5.65	-4.1	-5.96	-4	14	0.811	24.66	74.39	14.88	□
-5.32	-3.48	-5.65	-4.1	-5.96	-4	100	0.912	11.66	66.26	7.05	□
-5.34	-3.69	-6	-4	-5.75	-3.7	0	0.789	14.97	59.3	7.37	20
-5.34	-3.69	-6	-4	-5.75	-3.7	3	0.794	16.49	61.1	8.17	□
-5.34	-3.69	-6	-4	-5.75	-3.7	5	0.795	16.61	62.5	8.51	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.34	-3.69	-6	-4	-5.75	-3.7	10	0.801	14.01	55.1	6.83	□
-5.34	-3.69	-6	-4	-5.75	-3.7	100	1.136	4	44.5	2.13	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	0	0.83	13.3	58.5	6.74	21
-5.56	-3.67	-6	-4.15	-5.64	-4.04	10	0.86	13.9	63.6	7.92	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	20	0.87	14.8	63	8.18	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	30	0.87	14.5	55.5	7.24	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	40	0.88	11.5	53.3	5.6	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	50	0.89	8.28	42.1	3.31	□
-5.56	-3.67	-6	-4.15	-5.64	-4.04	100	0.97	10.27	51	5.43	□
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	0	0.796	16.73	63.81	8.5	22
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	5	0.808	17.08	66.95	9.24	□
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	10	0.814	17.56	67.51	9.65	□
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	15	0.82	17.82	67.54	9.87	□
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	20	0.826	17.62	63.94	9.31	□
-5.1	-3.3	-6.1	-4.3	-5.51	-3.91	25	0.832	17.29	60.55	8.71	□
-5.36	-3.39	-6.11	-4.3	-5.49	-3.45	0	0.93	13.95	69.6	9.05	23
-5.36	-3.39	-6.11	-4.3	-5.49	-3.45	20	0.93	14.62	74.2	10.14	□
-5.36	-3.39	-6.11	-4.3	-5.49	-3.45	100	0.9	13.56	65.3	8	□
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	0	0.8	12.13	54.99	5.34	24
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	5	0.83	11.76	58.89	5.75	□
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	10	0.82	11.62	62.54	5.96	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	15	0.83	12.57	62.93	6.56	□
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	20	0.82	10.22	65.72	5.51	□
-5.41	-3.53	-5.97	-3.98	-5.52	-3.7	30	0.84	9.35	66.05	5.19	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	0	0.879	17.28	72.7	11.04	25
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	9	0.882	17.74	75.7	11.84	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	17	0.892	18.19	75.1	12.19	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	23	0.893	18.1	74.1	11.98	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	29	0.901	17.76	73.2	11.71	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	38	0.898	17.69	73.5	11.67	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	50	0.893	17.64	71.3	11.23	□
-5.42	-3.41	-5.67	-4.02	-5.92	-3.9	100	0.914	12.28	78	8.75	□
-5.35	-3.62	-5.65	-3.96	-6.1	-4.1	0	0.97	19.54	59	11.18	26
-5.35	-3.62	-5.65	-3.96	-6.1	-4.1	25	0.89	21.91	68	13.26	□
-5.35	-3.62	-5.65	-3.96	-6.1	-4.1	100	0.84	12.5	63	6.62	□
-5.42	-3.61	-5.61	-4.08	-5.82	-3.94	0	0.851	20.62	74.7	13.11	27
-5.42	-3.61	-5.61	-4.08	-5.82	-3.94	9	0.849	21.48	75.29	13.73	□
-5.42	-3.61	-5.64	-4.1	-5.82	-3.94	0	0.865	25.26	71.4	15.6	27
-5.42	-3.61	-5.64	-4.1	-5.82	-3.94	9	0.866	25.57	73.84	16.35	□
-5.22	-3.64	-6	-4	-5.36	-3.55	0	0.78	17.5	66	9.2	28
-5.22	-3.64	-6	-4	-5.36	-3.55	10	0.79	19.14	67.7	10.4	□
-5.22	-3.64	-6	-4	-5.36	-3.55	100	0.8	4.33	37.1	1.3	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.22	-3.64	-6	-4	-5.47	-3.52	0	0.78	17.5	66	9.2	28
-5.22	-3.64	-6	-4	-5.47	-3.52	10	0.8	18.03	64.7	9.4	□
-5.22	-3.64	-6	-4	-5.47	-3.52	100	0.83	9.81	42.4	3.8	□
-5.22	-3.64	-6	-4	-5.41	-3.54	0	0.78	17.5	66	9.2	28
-5.22	-3.64	-6	-4	-5.41	-3.54	10	0.78	17.75	67.5	9.6	□
-5.22	-3.64	-6	-4	-5.41	-3.54	100	0.79	10.36	51.3	4.4	□
-5.29	-3.67	-6	-4	-5.24	-3.55	0	0.92	11.25	39	4.03	29
-5.29	-3.67	-6	-4	-5.24	-3.55	20	0.89	13.02	58	6.72	□
-5.07	-3.3	-5.65	-4.1	-6	-4	0	0.879	21.67	55.21	10.53	30
-5.07	-3.3	-5.65	-4.1	-6	-4	10	0.875	23	58.09	11.62	□
-5.07	-3.3	-5.65	-4.1	-6	-4	30	0.87	22.47	64.72	12.65	□
-5.07	-3.3	-5.65	-4.1	-6	-4	40	0.858	22.19	67.27	12.84	□
-5.07	-3.3	-5.65	-4.1	-6	-4	50	0.852	21.43	69.19	12.6	□
-5.07	-3.3	-5.65	-4.1	-6	-4	70	0.849	18.4	67.11	10.5	□
-5.07	-3.3	-5.65	-4.1	-6	-4	100	0.936	12.04	65.39	7.4	□
-5.24	-3.36	-5.44	-4.19	-5.96	-3.98	0	0.73	21.3	60	9.44	31
-5.24	-3.36	-5.44	-4.19	-5.96	-3.98	10	0.74	22.64	63	10.55	□
-5.24	-3.36	-5.44	-4.19	-5.96	-3.98	20	0.74	23.14	60	10.23	□
-5.24	-3.36	-5.44	-4.19	-5.96	-3.98	30	0.74	21.9	58	9.36	□
-5.24	-3.36	-5.44	-4.19	-5.96	-3.98	50	0.76	20.91	51	8.04	□
-5.3	-3.9	-5.67	-4.14	-6.1	-4.1	0	0.84	21.94	63	11.61	32



HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.3	-3.9	-5.67	-4.14	-6.1	-4.1	25	0.87	23.74	73	15.08	□
-5.3	-3.9	-5.67	-4.14	-6.1	-4.1	100	0.89	15.98	66	9.39	□
-5.5	-3.6	-5.9	-3.9	-5.5	-3.8	0	0.875	12.02	58.1	6.11	33
-5.5	-3.6	-5.9	-3.9	-5.5	-3.8	20	0.906	12.5	54.9	6.21	□
-5.5	-3.6	-5.9	-3.9	-5.5	-3.8	25	0.907	11.73	49.4	5.25	□
-5.22	-3.64	-5.65	-4.1	-5.96	-3.98	0	0.67	20.16	56.77	7.71	34
-5.22	-3.64	-5.65	-4.1	-5.96	-3.98	17	0.67	24.68	58.02	9.55	□
-5.22	-3.64	-5.65	-4.1	-5.96	-3.98	100	0.82	13.92	58.8	6.67	□
-5.36	-3.5	-6.02	-4.15	-5.5	-3.9	0	0.869	12.4	71.4	7.72	35
-5.36	-3.5	-6.02	-4.15	-5.5	-3.9	17	0.929	13	74.9	9.08	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	0	0.845	24.89	74.37	15.75	36
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	8	0.85	25.36	75.66	16.3	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	12.5	0.85	25.8	74.66	16.38	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	17	0.85	25.7	76.35	16.67	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	25	0.853	25.05	75.15	16.05	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	42	0.865	23.94	73.85	15.3	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	67	0.876	19.24	49.74	8.39	□
-5.5	-3.56	-5.7	-4.1	-5.92	-3.9	100	0.965	11.56	53.9	6.01	□
-4.9	-3	-6	-4	-5	-3.4	0	0.59	8.45	65	3.23	37
-4.9	-3	-6	-4	-5	-3.4	20	0.61	11.88	56.7	4.11	□
-4.9	-3	-6	-4	-5	-3.4	100	0.8	2.45	57.7	1.14	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.33	-3.43	-5.71	-4.18	-6	-4.12	0	0.89	19.91	72	12.81	38
-5.33	-3.43	-5.71	-4.18	-6	-4.12	15	0.9	20.82	73	13.67	□
-5.33	-3.43	-5.65	-4.29	-6	-4.12	0	0.84	24.99	72	15.05	38
-5.33	-3.43	-5.65	-4.29	-6	-4.12	15	0.85	25.96	74	16.43	□
-5.47	-3.67	-5.56	-4.03	-6	-3.9	0	0.9	19.49	69.73	12.23	39
-5.47	-3.67	-5.56	-4.03	-6	-3.9	33	0.92	19.86	73.2	13.37	□
-5.47	-3.67	-5.56	-4.03	-6	-3.9	50	0.92	18.48	72.71	12.36	□
-5.47	-3.67	-5.56	-4.03	-6	-3.9	60	0.92	17.83	71.48	11.72	□
-5.36	-3.54	-5.42	-4	-6	-3.9	0	0.9	21.87	58.7	11.55	40
-5.36	-3.54	-5.42	-4	-6	-3.9	33	0.88	23.7	64.2	13.38	□
-5.36	-3.54	-5.42	-4	-6	-3.9	50	0.88	23.8	64.4	13.49	□
-5.36	-3.54	-5.42	-4	-6	-3.9	60	0.88	23.78	63.9	13.37	□
-5.12	-3.6	-6.1	-3.9	-5.77	-3.68	0	0.804	15.68	67.7	8.53	41
-5.12	-3.6	-6.1	-3.9	-5.77	-3.68	3	0.804	17.15	68.4	9.43	□
-5.12	-3.6	-6.1	-3.9	-5.77	-3.68	6	0.807	16.39	65.9	8.72	□
-5.32	-3.77	-6	-4	-5.28	-3.48	0	0.94	14.06	58.56	7.74	42
-5.32	-3.77	-6	-4	-5.28	-3.48	10	0.92	15.64	63.59	9.15	□
-5.32	-3.77	-6	-4	-5.28	-3.48	20	0.9	15.98	65.72	9.45	□
-5.32	-3.77	-6	-4	-5.28	-3.48	30	0.9	15.15	63.37	8.64	□
-5.32	-3.77	-6	-4	-5.28	-3.48	40	0.89	14.66	59.02	7.7	□
-5.32	-3.77	-6	-4	-5.28	-3.48	100	0.85	13.16	67.94	7.6	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.39	-3.4	-5.52	-3.96	-5.94	-3.98	0	0.945	18.67	71.4	12.6	43
-5.39	-3.4	-5.52	-3.96	-5.94	-3.98	25	0.932	19.75	71.4	13.2	□
-5.45	-3.65	-5.6	-4.3	-6.1	-3.8	0	0.84	25.9	73	15.8	44
-5.45	-3.65	-5.6	-4.3	-6.1	-3.8	17	0.84	26	78	17	□
-5.33	-3.29	-5.51	-3.95	-6.1	-4	0	0.813	22.2	74	13.4	45
-5.33	-3.29	-5.51	-3.95	-6.1	-4	9	0.823	22.6	73.2	13.6	□
-5.33	-3.29	-5.51	-3.95	-6.1	-4	23	0.822	23.3	74.6	14.3	□
-5.33	-3.29	-5.51	-3.95	-6.1	-4	33	0.822	20.4	72.3	12.1	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	0	0.834	11.89	44.4	4.4	46
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	3	0.835	10.13	59.9	5.1	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	7	0.824	10.86	60.5	5.4	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	10	0.82	11.38	61.5	5.7	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	25	0.821	10.12	45.4	3.8	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	50	0.823	5.41	38.6	1.7	□
-5.02	-3.27	-6.1	-3.9	-5.24	-3.62	100	0.826	4.74	33.1	1.3	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	0	0.773	13.95	64	6.9	47
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	20	0.8	14.36	65.3	7.5	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	30	0.812	14.68	66.3	7.9	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	40	0.827	14.82	55.9	8.2	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	50	0.842	15.41	67.5	8.8	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	60	0.855	14.42	65.7	8.1	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	70	0.869	12.65	65.5	7.2	□
-5.12	-3.34	-6.1	-4.3	-5.21	-3.36	100	0.911	10.72	65.5	6.4	□
-5.32	-3.6	-5.61	-3.74	-6	-4	0	1.07	13.04	56	7.81	48
-5.32	-3.6	-5.61	-3.74	-6	-4	25	0.97	16.27	63	9.94	□
-5.32	-3.6	-5.61	-3.74	-6	-4	100	0.79	10.48	58	4.8	□
-5.39	-3.17	-5.51	-3.78	-5.96	-3.98	0	0.943	16.96	62.82	10.04	49
-5.39	-3.17	-5.51	-3.78	-5.96	-3.98	17	0.939	18.05	66.67	11.31	□
-5.39	-3.17	-5.51	-3.78	-5.96	-3.98	100	0.935	11.98	58.65	6.57	□
-5.26	-3.63	-6	-4.19	-5.35	-3.75	0	0.847	13.21	72.6	8.12	50
-5.26	-3.63	-6	-4.19	-5.35	-3.75	50	0.856	21.19	67.2	12.19	□
-5.26	-3.63	-6	-4.19	-5.35	-3.75	100	0.864	18.56	59.5	9.54	□
-5.36	-3.54	-5.49	-4.01	-6	-3.9	0	0.86	19.01	58.61	9.58	51
-5.36	-3.54	-5.49	-4.01	-6	-3.9	25	0.88	20.58	60.74	11	□
-5.36	-3.54	-5.49	-4.01	-6	-3.9	40	0.88	20.59	65.27	11.82	□
-5.36	-3.54	-5.49	-4.01	-6	-3.9	50	0.86	19.62	66.3	11.19	□
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	0	0.68	14.2	52.6	5.35	52
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	10	0.7	14.8	54.1	5.79	□
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	20	0.71	15.3	55.7	6.33	□
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	30	0.72	17.5	58.2	7.33	□
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	40	0.72	19.3	59.2	8.23	□
-5.15	-3.31	-6.1	-4.2	-6.1	-3.8	50	0.72	18.1	54.7	7.14	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.48	-3.52	-5.63	-3.97	-6	-3.9	0	0.89	19.8	59.05	10.43	53
-5.48	-3.52	-5.63	-3.97	-6	-3.9	20	0.9	20.04	59.69	10.71	□
-5.48	-3.52	-5.63	-3.97	-6	-3.9	35	0.89	20.75	60.94	11.26	□
-5.48	-3.52	-5.63	-3.97	-6	-3.9	50	0.88	19.17	57.53	9.68	□
-5.51	-3.3	-6	-4	-5.41	-3.38	0	0.73	15.3	65.25	7.2	54
-5.51	-3.3	-6	-4	-5.41	-3.38	10	0.74	16.7	64.14	8	□
-5.48	-3.64	-5.53	-3.83	-5.54	-3.87	0	0.89	17.24	70.98	10.9	55
-5.48	-3.64	-5.53	-3.83	-5.54	-3.87	15	0.9	18.1	70.81	11.55	□
-5.48	-3.64	-5.53	-3.83	-5.54	-3.87	30	0.89	19.29	70.18	12.36	□
-5.26	3.63	-5.5	-3.79	-6	-4.19	0	0.822	19.19	60.2	9.5	56
-5.26	3.63	-5.5	-3.79	-6	-4.19	20	0.829	19.14	65.6	10.41	□
-5	-3.4	-5.8	-4	-5.29	-3.31	0	0.795	16.67	63.7	8.44	57
-5	-3.4	-5.8	-4	-5.29	-3.31	6	0.811	16.81	63	8.59	□
-5	-3.4	-5.8	-4	-5.17	-3.16	6	0.802	17.26	65.6	9.08	57
-5.21	-2.99	-5.44	-4.19	-6.1	-3.9	0	0.675	22.27	61.3	9.21	58
-5.21	-2.99	-5.44	-4.19	-6.1	-3.9	20	0.69	22.6	65.7	10.26	□
-5.21	-2.99	-5.44	-4.19	-6.1	-3.9	40	0.698	22.7	67.4	10.68	□
-5.21	-2.99	-5.44	-4.19	-6.1	-3.9	60	0.713	19.67	69.3	9.73	□
-5.21	-2.99	-5.44	-4.19	-6.1	-3.9	100	0.723	10.15	69.7	5.12	□
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	0	0.86	15.7	71.6	9.65	59
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	20	0.87	16.8	72.11	10.67	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	40	0.88	16.35	71.21	10.27	□
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	60	0.88	15.76	69.78	9.78	□
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	80	0.87	15.18	69.46	9.24	□
-5.33	-2.92	-5.72	-3.85	-5.96	-3.98	100	0.86	13.3	64.67	7.47	□
-5.2	-3.3	-6.1	-3.9	-4.9	-4.2	0	0.73	14.48	47	4.98	60
-5.2	-3.3	-6.1	-3.9	-4.9	-4.2	25	0.64	11.15	23	1.57	□
-5.2	-3.3	-6.1	-3.9	-4.9	-4.2	50	0.77	15.31	52	6.02	□
-5.2	-3.3	-6.1	-3.9	-4.9	-4.2	100	0.71	15.21	50	5.48	□
-5.36	-3.54	-5.37	-3.73	-6	-3.9	0	1	12.69	57.6	7.31	61
-5.36	-3.54	-5.37	-3.73	-6	-3.9	33	0.9	15.55	52.7	7.38	□
-5.36	-3.54	-5.37	-3.73	-6	-3.9	50	0.88	16.78	56.4	8.32	□
-5.36	-3.54	-5.37	-3.73	-6	-3.9	60	0.84	17.03	56.4	8.29	□
-5.36	-3.54	-5.43	-3.94	-6	-3.9	0	0.88	15.19	56.3	7.52	61
-5.36	-3.54	-5.43	-3.94	-6	-3.9	33	0.86	16.97	61.8	9.01	□
-5.36	-3.54	-5.43	-3.94	-6	-3.9	50	0.84	16.98	61.9	8.83	□
-5.36	-3.54	-5.43	-3.94	-6	-3.9	60	0.84	17.79	61.4	9.18	□
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	0	0.83	9.47	47.77	3.75	62
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	9	0.84	9.74	49.43	4.04	□
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	23	0.84	10.19	50.76	4.35	□
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	33	0.85	10.12	51.64	4.44	□
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	41	0.85	10.86	51.98	4.8	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	50	0.87	10.46	50.92	4.64	□
-5.1	-3.4	-6.1	-4.3	-5.5	-3.6	100	0.87	6.52	57.59	3.27	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	0	0.778	16.21	60.1	7.58	63
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	3.3	0.8	16.33	64.8	8.46	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	6.7	0.795	17.21	64.3	8.8	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	13.3	0.792	17.5	60.6	8.4	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	26.7	0.788	18.53	55.5	8.1	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	40	0.787	18.12	48.9	6.98	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	60	0.735	5.51	29.1	1.18	□
-5.22	-3.64	-6.1	-4.3	-5.51	-4.08	5	0.803	19	61.6	9.48	□
-5.24	-3.61	-6	-4	-5.54	-2.79	0	0.77	18.39	65.49	9.26	64
-5.24	-3.61	-6	-4	-5.54	-2.79	5	0.77	18.66	66.13	9.59	□
-5.24	-3.61	-6	-4	-5.54	-2.79	10	0.78	19.14	67.26	10.05	□
-5.24	-3.61	-6	-4	-5.54	-2.79	15	0.78	19.45	67.61	10.27	□
-5.24	-3.61	-6	-4	-5.54	-2.79	20	0.78	18.14	67.35	9.49	□
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	0	0.836	11.99	67.54	6.77	65
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	30	0.863	13.98	67.26	8.16	□
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	50	0.871	15.29	68.29	9.1	□
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	70	0.897	15.51	67.74	9.43	□
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	80	0.915	16.44	67.58	10.17	□
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	90	0.926	15.44	69.07	9.87	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.33	-3.53	-6.1	-4.3	-5.58	-3.98	100	0.93	14.59	65.7	8.88	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	0	0.868	24.98	71.42	15.49	66
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	8	0.868	25.33	73.93	16.25	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	14	0.868	25.44	75.66	16.71	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	20	0.868	25.28	74.23	16.29	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	29	0.868	24.9	72.27	15.62	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	45	0.868	23.9	68.29	14.17	□
-5.51	-3.71	-5.65	-4.1	-5.96	-3.98	100	0.97	11.73	63.83	7.28	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	0	0.88	13.52	74.9	8.9	67
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	10	0.896	14.97	76.5	10.26	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	20	0.901	12.67	74.7	8.52	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	40	0.895	12.56	61.5	6.92	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	60	0.902	12.38	58.4	6.52	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	80	0.92	11.24	54.7	5.66	□
-5.02	-3.27	-6.1	-3.9	-5.22	-3.46	100	0.944	10.85	68.2	6.99	□
-5.24	-3.66	-5.42	-4.17	-6.19	-4	0	0.662	25.89	71.2	12.21	68
-5.24	-3.66	-5.42	-4.17	-6.19	-4	11	0.666	27.36	71.9	13.1	□
-5.24	-3.66	-5.42	-4.17	-6.19	-4	20	0.669	27.73	73	13.54	□
-5.24	-3.66	-5.42	-4.17	-6.19	-4	27	0.671	27.29	69	12.63	□
-5.2	-3.6	-6	-3.9	-5.7	-3.9	0	0.78	17.2	70	9.4	69
-5.2	-3.6	-6	-3.9	-5.7	-3.9	5	0.77	17.8	70	9.7	□



HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.2	-3.6	-6	-3.9	-5.7	-3.9	10	0.78	19.4	68	10.2	□
-5.2	-3.6	-6	-3.9	-5.7	-3.9	20	0.77	19.4	67	10	□
-5.2	-3.6	-6	-3.9	-5.7	-3.9	30	0.76	13.6	65	6.7	□
-5.2	-3.6	-6.1	-3.9	-5.28	-2.24	0	0.77	18.66	61.03	8.91	70
-5.2	-3.6	-6.1	-3.9	-5.28	-2.24	5	0.77	19.74	62.34	9.81	□
-5.2	-3.6	-6.1	-3.9	-5.28	-2.24	10	0.78	20.18	64.2	10.44	□
-5.2	-3.6	-6.1	-3.9	-5.28	-2.24	15	0.78	21.47	68.31	11.44	□
-5.2	-3.6	-6.1	-3.9	-5.28	-2.24	20	0.78	20.24	62.02	9.79	□
-5.24	-3.66	-6	-4	-5.19	-3.19	0	0.77	11.4	36.5	3.2	71
-5.24	-3.66	-6	-4	-5.19	-3.19	10	0.778	15	52	6.09	□
-5.44	-3.55	-6.19	-4	-5.49	-3.81	0	0.86	12.26	72	7.59	72
-5.44	-3.55	-6.19	-4	-5.49	-3.81	50	0.89	14.35	64	8.17	□
-5.44	-3.55	-6.19	-4	-5.38	-3.56	0	0.86	12.26	72	7.59	72
-5.44	-3.55	-6.19	-4	-5.38	-3.56	50	0.82	14.77	72	8.72	□
-5.22	-3.64	-5.44	-4.19	-5.96	-3.98	0	0.74	20.62	58.55	8.96	73
-5.22	-3.64	-5.44	-4.19	-5.96	-3.98	6	0.74	23.63	58	10.15	□
-5.54	-3.65	-5.56	-3.95	-5.96	-3.98	0	0.877	24.4	70.4	15.1	74
-5.54	-3.65	-5.56	-3.95	-5.96	-3.98	17	0.881	25.1	72.6	16.1	□
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	0	0.846	22.13	57.67	10.8	75
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	20	0.855	22.45	58.93	11.31	□
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	30	0.859	22.21	62	11.82	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	40	0.86	21.11	62.52	11.35	□
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	50	0.863	19.18	64.13	10.62	□
-5.3	-3.5	-5.6	-4.1	-6.1	-4.2	100	0.955	8.08	63.53	4.9	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	0	0.88	17.15	71.6	10.8	76
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	9	0.89	17.55	72.92	11.39	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	17	0.9	18.42	74.61	12.37	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	20	0.91	18.49	74.92	12.61	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	23	0.91	18.23	74.3	12.33	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	33	0.92	17.5	71.82	11.56	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	50	0.93	16.7	65.6	10.19	□
-5.68	-3.71	-5.74	-4.1	-6.1	-3.98	100	0.94	13.23	64	7.96	□
-5.13	-3.48	-5.34	-3.81	-6.1	-4.1	0	0.88	13.86	61	7.44	77
-5.13	-3.48	-5.34	-3.81	-6.1	-4.1	20	0.82	16.04	68	8.94	□
-5.13	-3.48	-5.34	-3.81	-6.1	-4.1	100	0.69	12.46	59	5.07	□
-5.5	-3.6	-6	-4	-5.8	-3.9	0	0.92	12.59	67	7.38	78
-5.5	-3.6	-6	-4	-5.8	-3.9	30	0.91	13.01	69	8.11	□
-5.5	-3.6	-6	-4	-5.8	-3.9	100	0.89	12.26	63	7.34	□
-5.38	-3.3	-5.54	-3.7	-6.1	-4.3	0	1.04	20.38	62	13.14	79
-5.38	-3.3	-5.54	-3.7	-6.1	-4.3	25	0.97	22.65	71	15.6	□
-5.38	-3.3	-5.54	-3.7	-6.1	-4.3	100	0.89	11.22	67	6.69	□
-5.39	-3.57	-5.69	-3.91	-5.79	-3.85	0	0.87	17.65	71.5	11.02	80

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.39	-3.57	-5.69	-3.91	-5.79	-3.85	10	0.89	18.69	70.88	11.86	□
-5.39	-3.57	-5.69	-3.91	-5.79	-3.85	20	0.89	19.41	64.14	11.08	□
-5.39	-3.57	-5.69	-3.91	-5.79	-3.85	50	0.91	16.06	64.49	9.45	□
-5.39	-3.57	-5.69	-3.91	-5.79	-3.85	100	0.93	12.63	61.96	7.28	□
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	0	0.84	10.87	57.1	5.28	81
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	10	0.87	11.5	61	6.21	□
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	15	0.88	12.01	63	6.73	□
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	20	0.86	11.63	62.8	6.39	□
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	30	0.84	11.22	59.4	5.62	□
-5.4	-3.55	-5.96	-4.26	-5.49	-3.9	100	0.8	5.91	60.9	2.93	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	0	0.87	12	53.2	5.7	82
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	25	0.87	14.2	54	7	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	37.5	0.87	12.9	53.2	6.1	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	50	0.91	12.1	53.4	6.1	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	62.5	0.91	11.2	52.5	5.6	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	71	0.94	10.1	50.5	4.9	□
-5.36	-3.52	-5.96	-3.98	-5.51	-3.78	100	0.97	8.3	49	4.2	□
-5.11	-3.4	-5.82	-4.18	-5.91	-4.1	0	0.87	15.2	64	8.7	83
-5.11	-3.4	-5.82	-4.18	-5.91	-4.1	29	0.87	16.3	72	10.8	□
-5.11	-3.4	-5.82	-4.18	-5.91	-4.1	41	0.86	16.4	70	10.3	□
-5.11	-3.4	-5.82	-4.18	-5.91	-4.1	50	0.85	16.4	69	9.9	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.11	-3.4	-5.82	-4.18	-5.91	-4.1	67	0.81	14.1	60	7.2	□
-5.22	-3.64	-6.1	-3.9	-5.43	-3.33	0	0.82	16.4	71.2	9.5	84
-5.22	-3.64	-6.1	-3.9	-5.43	-3.33	5	0.82	16	72	9.8	□
-5.22	-3.64	-6.1	-3.9	-5.43	-3.33	10	0.82	17.3	72.2	10.3	□
-5.22	-3.64	-6.1	-3.9	-5.43	-3.33	15	0.83	16.5	68	9.3	□
-5.22	-3.64	-6.1	-3.9	-5.43	-3.33	100	0.83	11.8	68	7.5	□
-5.2	-3.3	-6	-4.3	-5.3	-3.5	0	0.75	14.12	64.83	6.86	85
-5.2	-3.3	-6	-4.3	-5.3	-3.5	3	0.75	14.86	67.01	7.47	□
-5.2	-3.3	-6	-4.3	-5.3	-3.5	6	0.75	15.29	69.09	7.92	□
-5.2	-3.3	-6	-4.3	-5.3	-3.5	9	0.75	14.55	66.12	7.22	□
-5.2	-3.3	-6	-4.3	-5.3	-3.5	12	0.75	14.01	63.3	6.65	□
-5.2	-3.3	-6	-4.3	-5.3	-3.5	100	0.77	8.28	35.92	2.29	□
-5.4	-3.8	-6.1	-4.3	-5.6	-3.6	0	0.81	14.05	52.01	5.98	86
-5.4	-3.8	-6.1	-4.3	-5.6	-3.6	10	0.8	15.93	62.2	8.2	□
-5.4	-3.8	-6.1	-4.3	-5.6	-3.6	20	0.8	15.5	66.92	8.4	□
-5.4	-3.8	-6.1	-4.3	-5.6	-3.6	30	0.8	15.4	69.08	8.64	□
-5.4	-3.8	-6.1	-4.3	-5.6	-3.6	40	0.8	15.15	68.05	8.46	□
-5.15	-3.3	-6	-4.3	-5.66	-4.13	0	0.76	16.2	61.8	7.61	87
-5.15	-3.3	-6	-4.3	-5.66	-4.13	1	0.76	16.54	63	7.92	□
-5.15	-3.3	-6	-4.3	-5.66	-4.13	2	0.76	17.21	64	8.37	□
-5.15	-3.3	-6	-4.3	-5.66	-4.13	3	0.76	16.53	62.4	7.84	□

HOMO(D)	LUMO(D)	HOMO(A)	LUMO(A)	HOMO(T)	LUMO(T)	T(%)	Voc	Jsc	FF	PCE	Ref
-5.34	-3.69	-6	-4	-5.4	-3.27	0	0.75	19.5	72.2	10.57	88
-5.34	-3.69	-6	-4	-5.4	-3.27	5	0.76	19.2	74.3	10.89	□
-5.34	-3.69	-6	-4	-5.4	-3.27	10	0.77	19	75.1	11.07	□
-5.34	-3.69	-6	-4	-5.4	-3.27	15	0.79	18.8	74.7	11.17	□
-5.34	-3.69	-6	-4	-5.4	-3.27	20	0.81	17.9	73.1	10.56	□
-5.34	-3.69	-6	-4	-5.4	-3.27	30	0.82	16.2	67.1	9.1	□
-5.33	-3.29	-5.41	-3.97	-6	-4	0	0.85	21.3	66.9	12.1	89
-5.33	-3.29	-5.41	-3.97	-6	-4	13	0.857	22.8	71.6	14	□
-5.33	-3.29	-5.41	-3.97	-6	-4	23	0.858	20.2	67.3	11.6	□
-5.24	-3.66	-6	-4	-5.49	-4.04	0	0.81	15.2	69.6	8.6	90
-5.24	-3.66	-6	-4	-5.49	-4.04	17	0.82	14.3	53	6.2	□
-5.24	-3.66	-6	-4	-5.49	-4.04	33	0.82	14	52.5	6	□
-5.24	-3.66	-6	-4	-5.49	-4.04	50	0.83	12.3	52	5.3	□
-5.24	-3.66	-6	-4	-5.49	-4.04	67	0.8	9.3	49.1	3.7	□
-5.24	-3.66	-6	-4	-5.49	-4.04	100	0.8	10.4	56.5	4.7	□