

Table S-1 Crystallographic Data of **7a** and **8a**

	7a	8a
Crystal system	monoclinic	orthorhombic
Lattice type	primitive	primitive
space group	P21/c	P ₂₁₂₁₂₁
Lattice parameters		
a/Å	8.3237	7.8659
b/Å	7.8562	8.2045
c/Å	19.992	22.045
b/deg	101.266	-
V/Å ³	1282.12	1422.70
Z	4	4

Table S-2 FMO-TDDFT pair contribution analysis of **7a** and **8a** in S_0 and S_1 state

7a				8a			
Fragme nt index	S_0 - S_1 (e V)	Fragme nt index	S_1 - S_0 (e V)	Fragme nt index	S_0 - S_1 (e V)	Fragme nt index	S_1 - S_0 (e V)
1	3.875	1	3.076	1	4.031	1	3.167
3	-0.001	3	-0.004	3	-0.002	3	-0.003
4	0.002	4	-0.005	4	-0.015	4	0.009
5	-0.002	6	0.015	9	0.010	5	-0.038
7	-0.006	10	-0.025	15	0.004	9	0.022
11	-0.018	11	-0.027	17	0.001	10	0.006
12	-0.033	12	-0.005	18	-0.002	12	-0.004
13	-0.017	13	0.003	22	-0.015	16	-0.003
14	0.040	16	-0.003	23	-0.008	17	-0.003
18	-0.001	17	-0.003	24	-0.002	18	0.002
21	-0.004	18	-0.006	27	0.030	23	0.001
22	-0.009	20	-0.004	28	-0.059	24	-0.001
23	0.013	21	-0.006			25	0.002
24	-0.016	22	-0.001			26	-0.003
28	-0.007	26	-0.002			27	-0.001
32	-0.005	28	-0.009			28	0.015
		32	-0.006			29	-0.045
Total	3.810		2.986		3.940		3.124