Table S1

The electronic density, ρ(r), its corresponding Laplacian, $\nabla^2\rho(r)$, and electronic density energy, H(r), at hydrogen bond critical points (HBCPs) for the **6MQz-AC** and [6MQc][Y2-6], (Y2-6 = $CF_3CO_2^-$, BF_4^-, $CF_3SO_3^-$, $N(CF_3SO_2)_2^-$ and PF_6^-) at PBE0/6-311++G(d, p) level of theory.

	ρ(r)	$\nabla^2\rho(r)$	H(r)
6MQz-AC			
C7H17···O24	0.0102	0.0312	0.0010
H22–O23	0.2570	-1.4653	-0.4417
C7–H17	0.2848	-1.0090	-0.2845
O12···H22–O23	0.0970	0.1399	-0.0405
[6MQc][Y2]			
C7H17···O24	0.0161	0.0493	0.0015
O12H22···O23	0.0619	0.1428	–0.0139
C7–H17	0.2850	–1.0297	–0.2863
O12–H22	0.3042	-2.1008	-0.5920
[6MQc][Y3]			
C7H17···F24	0.0103	0.0365	0.0143
C7H17···F23	0.0067	0.0274	0.0012
O12H22···F23	0.0374	0.1362	-0.0010
C7–H17	0.2862	-1.0326	-0.2877
O12–H22	0.3399	-2.4928	-0.6836
[6MQc][Y4]			
C7H17···O24	0.0128	0.0396	0.0012
O12H22···O23	0.0453	0.1390	-0.0043
C7–H17	0.2860	-1.0304	-0.2872
O12–H22	0.3286	-2.3696	-0.6550
[6MQc][Y5]			
O12H22···O23	0.0356	0.1272	-0.0001
C7–H17···O23	0.0105	0.0370	0.0013
C7–H17…O24	0.0127	0.0477	0.0020
C7–H17	0.2872	-1.0419	-0.2896
O12–H22	0.3422	-2.4966	-0.6857
[6MQc][Y6]			
C7H17···F24	0.0098	0.0353	0.0012
C7H17···F23	0.0056	0.0237	0.0011
O12H22···F23	0.0298	0.1180	0.0010

C7–H17	0.2866	-1.0090	-0.2880
O12–H22	0.3482	-2.5664	-0.7016

Table S2. The calculated absorption wavelengths, oscillator strength, *f,* composition of the low-lying singlet excited states, and percentage of composition index (CI%) for the **[X][Y2-6],** (X = 6MQc$^+$, Y1-6 = $CH_3CO_2^-$, $CF_3CO_2^-$, BF_4^-, $CF_3SO_3^-$, $N(CF_3SO_2)_2^-$ and PF_6^-) in solution (Water, Acetonitrile, and Cyclohexene) at PBE0/6-311++G(d,p) level of theory

	Transition	λ (nm)	*f*	Composition	CI (%)
[X]$^+$		water			
	$S_0 \rightarrow S_1$	348.30	0.0646	H→L	96.50
	$S_0 \rightarrow S_2$	287.81	0.1077	H-1→L	79.22
				H→L+1	18.46
	$S_0 \rightarrow S_3$	230.94	0.6965	H-1→L	16.50
				H-1→L+2	4.88
				H→L+1	69.6
				H→L+2	6.51
[X]	$S_0 \rightarrow S_1$	488.21	0.0855	H→L	97.76
	$S_0 \rightarrow S_2$	380.87	0.0000	H-1→L	98.25
	$S_0 \rightarrow S_3$	309.52	0.0076	H-2→L	49.67
				H→L+1	48.95
[X][Y1]	$S_0 \rightarrow S_1$	454.97	0.1021		97.35
	$S_0 \rightarrow S_2$	330.41	0.0000	H–1→L	97.63
	$S_0 \rightarrow S_3$	304.62	0.0053	H–2→L	55.48
				H→L+1	28.49
[X][Y2]	$S_0 \rightarrow S_1$	551.47	0.0568	H→L	98.50
	$S_0 \rightarrow S_2$	354.21	0.0000	H-1→L	98.41
	$S_0 \rightarrow S_3$	314.45	0.0176	H-1→L	60.84
				H→L+1	18.88
				H→L+2	18.37
[X][Y3]	$S_0 \rightarrow S_1$	360.39	0.0727	H→L	95.67
	$S_0 \rightarrow S_2$	293.60	0.1063	H-1→L	78.95
				H→L+1	17.88

	$S_0 \rightarrow S_3$	236.54	0.6946	H-1→L	15.74
				H→L+2	3.79
				H→L+1	72.89
				H→L+2	2.4
[X][Y4]	$S_0 \rightarrow S_1$	369.29	0.0792	H→L	96.24
	$S_0 \rightarrow S_2$	293.31	0.0960	H-1→L	77.14
				H→L+1	20.02
	$S_0 \rightarrow S_3$	251.91	0.0026	H-2→L	98.60
[X][Y5]	$S_0 \rightarrow S_1$	348.73	0.0562	H-1→L	14.04
				H→L	95.45
	$S_0 \rightarrow S_2$	297.37	0.1217	H-1→L	82.33
				H→L+1	14.41
	$S_0 \rightarrow S_3$	248.27	0.0097	H-2→L	92.33
				H→L+1	4.75
[X][Y6]	$S_0 \rightarrow S_1$	348.73	0.0562	H→L	97.73
	$S_0 \rightarrow S_2$	297.37	0.1217	H-1→L	76.17
				H→L+1	9.98
	$S_0 \rightarrow S_3$	248.27	0.0097	H-1→L	15.65
				H-1→L+2	3.51
				H→L+1	31.36
				H→L+2	15.53

	Transition	λ (nm)	*f*	Composition	CI (%)
		Acetonitrile			
$[X]^+$	$S_0 \rightarrow S_1$	348.89	348.89	H→L	96.51
	$S_0 \rightarrow S_2$	287.96	0.1085	H-1→L	79.28
				H→L+1	18.41
	$S_0 \rightarrow S_3$	231.18	0.7010	H-1→L	16.48
				H-1→L+2	4.82
				H→L+1	69.90
				H→L+2	6.36
[X]	$S_0 \rightarrow S_1$	491.39	0.0861	H→L	97.77
	$S_0 \rightarrow S_2$	383.81	0.0000	H-1→L	98.26
	$S_0 \rightarrow S_3$	310.12	0.0080	H-2→L	49.32
				H→L+1	49.33
[X][Y1]	$S_0 \rightarrow S_1$	509.67	0.1034	H→L	97.3
	$S_0 \rightarrow S_2$	379.71	0.0000	H−1→L	97.18
	$S_0 \rightarrow S_3$	316.59	0.0072	H−3→L	51.93
				H→L+1	46.76
[X][Y2]	$S_0 \rightarrow S_1$	641.07	0.0556	H→L	98.64
	$S_0 \rightarrow S_2$	410.26	0.0000	H-1→L	98.63

	$S_0 \rightarrow S_3$	327.71	0.0112	H-2→L	59.42
				H→L+1	38.91
[X][Y3]	$S_0 \rightarrow S_1$	393.84	0.0751	H-1→L	33.70
				H→L	95.09
	$S_0 \rightarrow S_2$	306.40	0.1117	H-1→L	79.63
				H→L	2.21
				H→L+1	16.50
	$S_0 \rightarrow S_3$	247.71	0.6699	H-1→L	14.47
				H-1→L+2	2.62
				H→L+1	77.80
[X][Y4]	$S_0 \rightarrow S_1$	404.63	0.0824	H-2→L	2.41
				H→L	95.81
	$S_0 \rightarrow S_2$	341.71	0.0034	H-1→L	99.30
	$S_0 \rightarrow S_3$	304.89	0.0934	H-3→L	2.21
				H-2→L	75.27
				H→L+1	19.11
[X][Y5]	$S_0 \rightarrow S_1$	349.75	0.0564	H-1→L	2.07
				H→L	95.42
	$S_0 \rightarrow S_2$	297.92	0.1228	H-1→L	82.44
				H→L+1	14.23
	$S_0 \rightarrow S_3$	250.22	0.0071	H-2→L	92.91
				H→L+1	4.28
[X][Y6]	$S_0 \rightarrow S_1$	437.13	0.0578	H→L	97.73
	$S_0 \rightarrow S_2$	300.22	0.1007	H-1→L	78.48
				H→L	19.62
	$S_0 \rightarrow S_3$	244.10	0.5747	H-1→L	7.95
				H-1→L+2	3.39
				H→L+1	32.47
				H→L+2	13.36

	Transition	λ (nm)	*f*	Composition	CI (%)
		Cyclohexane			
$[X]^+$	$S_0 \rightarrow S_1$	361.56	0.0658	H→L	96.69
	$S_0 \rightarrow S_2$	290.83	0.1091	H-1→L	79.26
				H→L+1	18.38
	$S_0 \rightarrow S_3$	234.92	0.7314	H-1→L	16.70
				H-1→L+2	4.20
				H→L+1	72.33
				H→L+2	4.73
[X]	$S_0 \rightarrow S_1$	488.21	0.0855	H→L	97.76

	$S_0 \rightarrow S_2$	380.87	0.0000	H-1→L	98.25
	$S_0 \rightarrow S_3$	309.52	0.0076	H-2→L	49.67
				H→L+1	48.95
[X][Y1]	$S_0 \rightarrow S_1$	509.67	0.1034	H→L	97.32
	$S_0 \rightarrow S_2$	379.71	0.0000	H–1→L	97.19
	$S_0 \rightarrow S_3$	316.59	0.0072	H–3→L	51.93
				H→L+1	46.76
[X][Y2]	$S_0 \rightarrow S_1$	641.07	0.0556	H→L	98.64
	$S_0 \rightarrow S_2$	410.26	0.0000	H-1→L	98.63
	$S_0 \rightarrow S_3$	327.71	0.0112	H-2→L	52.41
				H→L+1	38.91
[X][Y3]	$S_0 \rightarrow S_1$	393.84	0.0751	H-1→L	3.27
				H→L	95.09
	$S_0 \rightarrow S_2$	306.40	0.1117	H-1→L	79.63
				H→L	2.21
				H→L+1	16.49
	$S_0 \rightarrow S_3$	247.71	0.6699	H-1→L	14.47
				H-1→L+2	2.61
				H→L+1	77.79
[X][Y4]	$S_0 \rightarrow S_1$	402.02	0.0892	H-2→L	2.36
				H-1→L	2.44
				H→L	93.57
	$S_0 \rightarrow S_2$	347.81	0.0351	H-1→L	95.18
				H→L	2.85
	$S_0 \rightarrow S_3$	304.51	0.0774	H-2→L	78.87
				H→L+1	15.71
[X][Y5]	$S_0 \rightarrow S_1$	373.46	0.0565	H-2→ L	2.15
				H-1→L	2.35
				H→L	93.59
	$S_0 \rightarrow S_2$	321.90	0.0683	H-2→L	3.54
				H-1→L	88.95
				H→L	2.97
				H→L+1	3.89
	$S_0 \rightarrow S_3$	299.11	0.0623	H-2→L	80.63
				H-1→L	7.15
				H→L+1	9.62
[X][Y6]	$S_0 \rightarrow S_1$	488.25	0.0551	H→L	97.61
	$S_0 \rightarrow S_2$	313.58	0.0978	H-1→L	78.88
				H→L+1	19.02
	$S_0 \rightarrow S_3$	254.67	0.6540	H-1→L	16.54
				H-1→L+2	2.75
				H→L+1	72.93

H→L+2	5.60