

## Supplementary Information for

# Tartrate-stabilized titanium-oxo clusters containing sulfonate chromophore ligands: Synthesis, crystal structures and photochemical properties

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**Figure S8** (a) The hydrogen bonds between adjacent TOCs of **2**; (b) The 3D supramolecular network of **2** viewing along *a*-axis. The most hydrogen atoms are omitted for clarity.

**Table S1** Geometrical parameter of **1** and **2**: Internal coordinates at DFT/B3LYP method with 6-311G\* and LANL2DZ basis set.

<b>1</b>			
Ti	-2.47259179	1.05778797	1.70748006
Ti	-2.97394888	1.26918024	-1.46357550
S	-3.13418241	-1.77612933	-0.12147738
O	-1.35724250	0.49405939	-2.51071701
O	-1.52806234	0.95595958	-0.04498077
O	0.72785215	-0.27297759	-2.46209409
O	-2.88977625	-1.10857170	1.19717774
O	-3.85930627	1.46605199	0.34316446
O	-3.48117673	-0.77169970	-1.19096136
O	-1.97433199	2.72409205	2.11694407
O	-2.03551685	-2.66542858	-0.54414468
O	-4.18202873	1.40098527	-2.77237834
O	-3.42776256	0.67969149	3.16456679
O	-2.39238474	2.95788929	-1.64901970
N	-4.16340008	-3.98376612	-1.98025246
H	-4.35725589	-4.83417797	-2.48289252
H	-3.18701257	-3.72628738	-1.93726933
C	-0.28263575	0.23003909	-1.90548377
C	-4.59200599	-2.76353623	0.09483143
C	-4.93014917	-3.74158044	-0.86699276
C	-0.24437374	0.58805737	-0.42460163
H	0.44229897	1.42813181	-0.29828578
C	-6.93976697	-4.18233608	0.43811683
H	-7.85917455	-4.74535205	0.56158094
C	-5.40088625	-2.51309179	1.20159260
H	-5.08119957	-1.76243605	1.91219822
C	-6.13504417	-4.44060442	-0.65860542
H	-6.42843850	-5.19665373	-1.38091754
C	-6.58016362	-3.21949303	1.38419132
H	-7.20706631	-3.02650016	2.24655613
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H	-5.31482483	1.79054610	1.72423743
C	-6.20916639	1.00459600	-0.06355346
H	-6.09067181	1.06165560	-1.14652150
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H	-1.03341392	3.37613381	-0.18458770

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H	0.29196413	4.01829007	4.21243581
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C	-0.21509623	3.86623044	-2.11991315
H	0.18707055	2.87445637	-2.32640064
H	0.59757886	4.47224799	-1.71228023
H	-0.54366737	4.30223656	-3.06728109
C	-3.76528309	1.50314419	-5.12283832
H	-2.69940408	1.36205143	-4.93512882
H	-3.88653319	2.10609580	-6.02747354
H	-4.21356852	0.52103529	-5.29358270
C	-3.89210370	-0.15988270	4.20309358
H	-4.85233792	-0.57754705	3.86971710
C	-5.92903594	2.36109134	-4.09519780
H	-6.41344384	1.38960357	-4.22261562
H	-6.15004856	2.97724763	-4.97117228
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H	-2.36678840	5.61278628	-1.78949550
H	-1.22722629	5.85478549	-0.45087144
H	-2.80039017	5.09935766	-0.14919033
C	-2.11540599	4.89085355	3.10425233
H	-1.69196528	5.36875794	2.21783674
H	-1.86192617	5.49549446	3.97955652
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C	-4.12681844	0.69212454	5.44573878
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H	-4.56165178	0.09348255	6.25092906
H	-4.80544544	1.51810992	5.22185334
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H	-2.77481944	-1.88370634	3.52906930
H	-3.25644957	-1.94983263	5.23894456
H	-1.92622973	-0.89230488	4.71762671
C	-5.33687697	3.37293472	0.27400124
H	-4.58076865	3.96091083	0.79595324
H	-6.32555877	3.74892741	0.55163735
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O	-0.72785620	0.27292993	2.46209564
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O	3.85932607	-1.46603372	-0.34316270
O	3.48113804	0.77170986	1.19096336
O	1.97438003	-2.72411503	-2.11694651
O	2.03546327	2.66542553	0.54414220
O	4.18204222	-1.40095795	2.77238272
O	3.42776227	-0.67968241	-3.16456773
O	2.39243442	-2.95790411	1.64902775
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C	4.59194778	2.76354763	-0.09484315
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H	5.08116113	1.76243314	-1.91219698
C	6.13496198	4.44064183	0.65858296
H	6.42834288	5.19670306	1.38088807
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H	7.20701582	3.02651782	-2.24655742
C	5.20433604	-1.90298210	-0.64163938
H	5.31485483	-1.79049409	-1.72423393
C	6.20917925	-1.00456374	0.06357505
H	6.09068017	-1.06164364	1.14654155
H	7.22740698	-1.31160472	-0.19220460
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C	1.57180275	-3.47587054	-3.25225585
H	2.01904826	-3.00250349	-4.13673214
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C	4.42562579	-2.18378506	3.92945226
H	3.95001987	-3.15909715	3.75539536
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H	-0.18702778	-2.87448608	2.32637590

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H	0.54371751	-4.30224305	3.06729422
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H	2.69941153	-1.36202931	4.93512906
H	3.88654925	-2.10604638	6.02748307
H	4.21356182	-0.52098664	5.29358048
C	3.89207984	0.15989876	-4.20309949
H	4.85231285	0.57757497	-3.86973440
C	5.92906139	-2.36102478	4.09521437
H	6.41345352	-1.38952814	4.22262456
H	6.15008190	-2.97716972	4.97119485
H	6.36048293	-2.84689143	3.21717653
C	1.98074137	-5.17790564	0.86360117
H	2.36686664	-5.61279808	1.78955734
H	1.22732202	-5.85483878	0.45092609
H	2.80048106	-5.09940050	0.14924601
C	2.11549629	-4.89087172	-3.10426309
H	1.69206929	-5.36878831	-2.21784767
H	1.86202519	-5.49551452	-3.97956852
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C	4.12678999	-0.69210401	-5.44574868
H	3.18044441	-1.11045327	-5.79837017
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H	4.80543034	-1.51808094	-5.22187262
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H	2.77478195	1.88370716	-3.52905883
H	3.25639016	1.94984185	-5.23894002
H	1.92619026	0.89229636	-4.71760701
C	5.33691443	-3.37290438	-0.27402177
H	4.58081402	-3.96087920	-0.79598646
H	6.32560100	-3.74888344	-0.55165932
H	5.20037532	-3.51841502	0.79975258

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**2**

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Ti	-3.01495769	-1.12999910	-1.35152900
Ti	-2.56079618	1.89723482	-0.31503240
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O	-1.55159123	0.20115272	-0.92473217
O	0.76850062	-2.43644584	-0.48874640
O	-1.31370045	-2.28910858	-1.23015978
O	-3.96163094	0.59637159	-0.94932381
O	-2.86672996	-1.41708276	0.85078900
O	-2.69817424	0.92546471	1.61003335
O	-2.06892323	2.74392115	-1.81077651
O	-3.01815887	-1.03102129	-3.13919128

O	-4.11634479	-2.52753291	-1.22619756
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O	-2.46720524	-0.95076884	3.22775225
C	-0.24953477	-1.76745134	-0.79936434
C	-4.87451656	-0.42295235	2.23714414
C	-5.56091140	0.75237580	1.93495136
H	-4.99181207	1.62583926	1.64064815
C	-0.25470309	-0.23947787	-0.68682798
H	0.41878495	0.13099292	-1.46457526
C	-5.54429762	-1.58800185	2.66279878
N	-4.87828932	-2.76317143	2.97292451
H	-5.41885229	-3.43593955	3.49424548
H	-3.93479699	-2.66093774	3.32235097
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C	-6.94801362	-1.52362237	2.70028349
H	-7.50481043	-2.40498437	3.00640963
C	-7.62623269	-0.36177151	2.36554734
H	-8.71208350	-0.35946992	2.40749057
C	-5.26487681	1.03567291	-1.42748551
H	-5.59717089	1.77921290	-0.69895141
C	-4.38209386	-3.68363194	-0.43750252
H	-4.02464705	-3.47324137	0.57351655
C	-3.21095324	-1.95205740	-4.20771615
H	-3.87148900	-2.74523743	-3.83017659
C	-6.23652110	-0.13359306	-1.42894422
H	-5.96218783	-0.88094965	-2.17560441
H	-7.24346322	0.22754783	-1.65580061
H	-6.25416397	-0.61702946	-0.45294747
C	-5.88825743	-3.90656857	-0.40133137
H	-6.39090856	-3.04439010	0.04084081
H	-6.12666279	-4.78801415	0.20096357
H	-6.27956215	-4.05890765	-1.41132644
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C	-0.63855414	4.17431879	-3.08902145
H	-1.47907942	4.54947507	-3.67969470
H	0.26560548	4.21841252	-3.70246118
H	-0.50368193	4.82587005	-2.22284930
C	-3.81160592	4.58198926	-0.03976205
H	-3.50292031	4.71464550	-1.08580223
C	-5.10206448	1.68701031	-2.79384783
H	-4.43993954	2.55154116	-2.73586251
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H	-4.65978199	0.97553990	-3.49234061

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H	-8.15271002	1.95619443	0.60807602
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C	-2.87105120	5.37210789	0.86467118
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H	-1.84585135	5.01974530	0.73540712
C	-1.09877706	1.76733316	-3.79321008
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C	-3.60315539	-4.85302625	-1.02988251
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H	-3.73569702	-5.75258824	-0.42138828
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C	-5.27440019	4.97085002	0.12534306
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H	-5.42863466	6.01971808	-0.14327651
H	-5.58854134	4.83201008	1.16329823
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H	-4.85565525	-0.82878178	-5.06208521
H	-4.03542214	-1.90050906	-6.20940537
H	-3.26045660	-0.38799577	-5.69610910
C	-1.85778588	-2.54975356	-4.58077024
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Ti	3.01497309	1.13000135	1.35153335
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O	1.55159180	-0.20118410	0.92480721
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O	1.31368609	2.28907949	1.23024229
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O	2.69809889	-0.92540379	-1.61005517
O	2.06901693	-2.74389193	1.81079282
O	3.01817850	1.03095421	3.13919059
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O	3.66430420	-3.19732219	-0.26139849
O	2.46724447	0.95087922	-3.22774244
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C	5.56085081	-0.75240882	-1.93499662
H	4.99172824	-1.62588378	-1.64076826
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N	4.87831259	2.76324892	-2.97263302
H	5.41889912	3.43603927	-3.49390786
H	3.93484338	2.66103324	-3.32213560
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C	7.62620887	0.36170895	-2.36549738
H	8.71205794	0.35937796	-2.40746123
C	5.26494825	-1.03560251	1.42732748
H	5.59724196	-1.77913942	0.69878934
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H	4.02439254	3.47342970	-0.57340191
C	3.21099812	1.95195345	4.20774637
H	3.87139545	2.74523140	3.83017414
C	6.23653793	0.13371529	1.42872824
H	5.96225472	0.88101499	2.17546123
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H	6.25403454	0.61720675	0.45275659
C	5.88804703	3.90680471	0.40134090
H	6.39071896	3.04467474	-0.04090055
H	6.12635423	4.78828896	-0.20093601
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C	0.90319354	-2.74413979	2.64140935
H	0.06226565	-2.40740600	2.02456286
C	0.63869616	-4.17446221	3.08889442
H	1.47925931	-4.54970945	3.67945749
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C	3.81157825	-4.58197315	0.03952866
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H	6.07341280	-2.01044244	3.17908015
H	4.65997211	-0.97544664	3.49221545
C	7.70126605	-2.05499236	-1.60209076
H	8.51306856	-2.27149678	-2.30224414
H	8.15097744	-1.95701479	-0.60729691
H	7.04193083	-2.92371786	-1.57587739
C	2.87092676	-5.37202746	-0.86486330

H	3.14811670	-5.23185681	-1.91307647
H	2.91156561	-6.43971754	-0.63006998
H	1.84574280	-5.01966593	-0.73547688
C	1.09895805	-1.76755272	3.79335696
H	1.41016607	-0.79454551	3.41632232
H	0.16064570	-1.64896811	4.34078190
H	1.87269776	-2.12931248	4.47700846
C	3.60293056	4.85306059	1.03014378
H	3.94649197	5.06767473	2.04661859
H	3.73538255	5.75268429	0.42172152
H	2.54050104	4.60698814	1.06763616
C	5.27435433	-4.97083054	-0.12575363
H	5.91092802	-4.35489196	0.51390408
H	5.42862154	-6.01970157	0.14283667
H	5.58837877	-4.83197445	-1.16374232
C	3.88327525	1.22290555	5.36439275
H	4.85596833	0.82888299	5.06187323
H	4.03564245	1.90036019	6.20936171
H	3.26089704	0.38776221	5.69598591
C	1.85779949	2.54946116	4.58098632
H	1.18082952	1.76423418	4.92795798
H	1.96888214	3.29194703	5.37657272
H	1.40642407	3.02941114	3.71147031

**Table S2** Bond lengths(Å) for complex **1**.

Bond	Distance(Å)	Bond	Distance(Å)	Bond	Distance(Å)
Ti1 - Ti2	3.2194(14)	S1 - O6	1.460(4)	C2 - C6	1.366(7)
Ti1 - O2	2.003(3)	S1 - O8	1.437(4)	C3 - C7	1.395(8)
Ti1 - O3 <sup>1</sup>	2.068(3)	S1 - C2	1.753(5)	C4 - C41	1.484(10)
Ti1 - O4	2.218(4)	O1 - C1	1.248(6)	C5 - C7	1.330(9)
Ti1 - O5	1.997(4)	O2 - C4	1.402(5)	C5 - C8	1.367(9)
Ti1 - O7	1.777(4)	O3 - C1	1.260(6)	C6 - C8	1.384(8)
Ti1 - O10	1.758(4)	O5 - C9	1.438(7)	C9 - C10	1.420(11)
Ti2 - O1	2.068(3)	O7 - C11	1.415(8)	C9 - C23	1.426(8)
Ti2 - O2	2.022(3)	O9 - C13	1.349(10)	C11 - C14	1.450(13)
Ti2 - O5	2.020(4)	O10 - C17	1.340(12)	C11 - C20	1.396(14)
Ti2 - O6	2.187(4)	O11 - C12	1.441(11)	C12 - C15	1.387(15)
Ti2 - O9	1.763(4)	N1 - C3	1.358(7)	C12 - C19	1.443(14)
Ti2 - O11	1.767(4)	C1 - C4	1.559(7)	C13 - C16	1.366(15)
S1 - O4	1.468(4)	C2 - C3	1.396(7)	C13 - C18	1.451(16)

**Table S3** Bond angles (°) for complex **1**.

Bond	Angles (°)	Bond	Angles (°)	Bond	Angles (°)
O2-Ti1-Ti2	37.08(9)	O9-Ti2-Ti1	143.42(15)	O1-C1-O3	123.9(4)
O2-Ti1-O3 <sup>1</sup>	83.24(13)	O9-Ti2-O1	98.43(18)	O1-C1-C4	113.6(4)
O2-Ti1-O4	80.95(14)	O9-Ti2-O2	168.44(18)	O3-C1-C4	122.4(4)
O3 <sup>1</sup> -Ti1-Ti2	119.54(10)	O9-Ti2-O5	109.24(18)	C3-C2-S1	120.2(4)
O3 <sup>1</sup> -Ti1-O4	83.80(13)	O9-Ti2-O6	84.32(17)	C6-C2-S1	119.2(4)
O4-Ti1-Ti2	79.06(10)	O9-Ti2-O11	97.7(2)	C6-C2-C3	120.6(5)
O5-Ti1-Ti2	36.98(10)	O11-Ti2-Ti1	99.77(16)	N1-C3-C2	122.8(5)
O5-Ti1-O2	73.88(13)	O11-Ti2-O1	93.81(17)	N1-C3-C7	120.4(5)
O5-Ti1-O3 <sup>1</sup>	156.15(15)	O11-Ti2-O2	93.13(18)	C7-C3-C2	116.7(5)
O5-Ti1-O4	85.98(14)	O11-Ti2-O5	98.20(19)	O2-C4-C1	109.5(4)
O7-Ti1-Ti2	102.47(15)	O11-Ti2-O6	177.28(18)	O2-C4-C4 <sup>1</sup>	110.7(5)
O7-Ti1-O2	96.94(18)	O4-S1-C2	105.3(2)	C4 <sup>1</sup> -C4-C1	109.5(5)
O7-Ti1-O3 <sup>1</sup>	90.73(16)	O6-S1-O4	110.8(2)	C7-C5-C8	121.3(6)
O7-Ti1-O4	174.32(17)	O6-S1-C2	107.4(2)	C2-C6-C8	120.7(6)
O7-Ti1-O5	98.53(17)	O8-S1-O4	114.3(2)	C5-C7-C3	122.2(6)
O10-Ti1-Ti2	137.54(14)	O8-S1-O6	111.1(3)	C5-C8-C6	118.5(6)
O10-Ti1-O2	164.48(19)	O8-S1-C2	107.4(2)	C10-C9-O5	113.6(6)
O10-Ti1-O3 <sup>1</sup>	96.40(18)	C1-O1-Ti2	120.9(3)	C10-C9-C23	133.5(8)
O10-Ti1-O4	83.59(19)	Ti1-O2-Ti2	106.25(13)	C23-C9-O5	112.4(7)
O10-Ti1-O5	103.81(18)	C4-O2-Ti1	135.4(3)	O7-C11-C14	111.0(8)
O10-Ti1-O7	98.6(2)	C4-O2-Ti2	118.0(3)	C20-C11-O7	111.7(9)
O1-Ti2-Ti1	112.11(10)	C1-O3-Ti1 <sup>1</sup>	130.8(3)	C20-C11-C14	117.3(10)
O1-Ti2-O6	84.08(14)	S1-O4-Ti1	133.1(2)	O11-C12-C19	113.5(10)
O2-Ti2-Ti1	36.67(9)	Ti1-O5-Ti2	106.55(15)	C15-C12-O11	114.2(11)
O2-Ti2-O1	76.73(13)	C9-O5-Ti1	128.0(5)	C15-C12-C19	118.8(13)
O2-Ti2-O6	84.73(13)	C9-O5-Ti2	125.4(5)	O9-C13-C16	121.0(11)
O5-Ti2-Ti1	36.48(10)	S1-O6-Ti2	132.2(2)	O9-C13-C18	115.7(11)
O5-Ti2-O1	147.88(14)	C11-O7-Ti1	140.5(5)	C16-C13-C18	119.9(12)
O5-Ti2-O2	72.97(13)	C13-O9-Ti2	159.1(7)	O10-C17-C21	120.0(12)
O5-Ti2-O6	82.79(15)	C17-O10-Ti1	164.5(7)	O10-C17-C22	114.5(11)
O6-Ti2-Ti1	79.50(9)	C12-O11-Ti2	142.2(6)	C21-C17-C22	124.5(13)

**Table S4** Bond lengths(Å) for complex **2**.

Bond	Distance(Å)	Bond	Distance(Å)	Bond	Distance(Å)
Ti1 - Ti2	3.2323(13)	O2 - C1	1.250(5)	C2 - C5	1.398(7)
Ti1 - O1	2.008(3)	O3 - C1	1.251(6)	C3 - C6	1.384(7)
Ti1 - O3	2.073(3)	O4 - C9	1.459(6)	C4 - C41	1.520(9)
Ti1 - O4	2.005(3)	O7 - C14	1.432(8)	C5 - N1	1.361(6)
Ti1 - O5	2.223(3)	O8 - C11	1.436(6)	C5 - C7	1.404(8)
Ti1 - O8	1.772(3)	O9 - C10	1.400(7)	C6 - C8	1.371(8)

Ti1 - O9	1.763(4)	O10 - C16	1.362(7)	C6 - C18	1.507(8)
Ti2 - O1	2.031(3)	C1 - C4	1.562(6)	C7 - C8	1.355(8)
Ti2 - O21	2.063(3)	C2 - C3	1.371(6)	C9 - C12	1.476(8)
Ti2 - O4	1.996(3)	C2 - C5	1.398(7)	C9 - C17	1.463(8)
Ti2 - O6	2.177(3)	C3 - C6	1.384(7)	C10- C13	1.492(8)
Ti2 - O7	1.742(4)	C4 - C41	1.520(9)	C10 - C21	1.483(8)
Ti2 - O10	1.785(3)	C5 - N1	1.361(6)	C11 - C23	1.483(8)
S1 - O5	1.468(3)	C5 - C7	1.404(8)	C11 - C24	1.478(9)
S1 - O6	1.465(3)	O9 - C10	1.400(7)	C14 - C15	1.504(8)
S1 - O11	1.432(3)	O10 - C16	1.362(7)	C14-C20	1.427(9)
S1 - C2	1.753(5)	C1 - C4	1.562(6)	C16-C19	1.474(9)
O1 - C4	1.404(5)	C2 - C3	1.371(6)	C16-C22	1.468(10)

**Table S5** Bond angles ( ° ) for complex **2**.

Bond	Angles ( ° )	Bond	Angles ( ° )	Bond	Angles ( ° )
O1-Ti1-Ti2	37.09(8)	O7-Ti2-O1	98.06(15)	O3-C1-C4	114.1(4)
O1-Ti1-O3	76.78(13)	O7-Ti2-O2 <sup>1</sup>	89.12(15)	C3-C2-S1	118.6(4)
O1-Ti1-O5	85.80(12)	O7-Ti2-O4	97.89(15)	C3-C2-C5	120.8(5)
O3-Ti1-Ti2	111.58(10)	O7-Ti2-O6	173.42(15)	C5-C2-S1	120.6(4)
O3-Ti1-O5	81.63(12)	O7-Ti2-O10	98.07(17)	C2-C3-C6	122.6(6)
O4-Ti1-Ti2	36.01(9)	O10-Ti2-Ti1	134.68(13)	O1-C4-C1	108.8(4)
O4-Ti1-O1	72.67(12)	O10-Ti2-O1	163.59(15)	O1-C4-C4 <sup>1</sup>	110.6(5)
O4-Ti1-O3	146.74(14)	O10-Ti2-O2 <sup>1</sup>	99.76(15)	C4 <sup>1</sup> -C4-C1	109.0(5)
O4-Ti1-O5	83.31(13)	O10-Ti2-O4	102.41(15)	C2-C5-C7	115.9(6)
O5-Ti1-Ti2	78.95(8)	O10-Ti2-O6	83.22(15)	N1-C5-C2	123.0(5)
O8-Ti1-Ti2	103.64(11)	O5-S1-C2	107.1(2)	N1-C5-C7	121.0(6)
O8-Ti1-O1	93.74(14)	O6-S1-O5	110.77(19)	C3-C6-C18	121.1(7)
O8-Ti1-O3	93.44(14)	O6-S1-C2	105.1(2)	C8-C6-C3	116.2(6)
O8-Ti1-O4	101.30(14)	O11-S1-O5	112.3(2)	C8-C6-C18	122.6(6)
O8-Ti1-O5	175.02(14)	O11-S1-O6	113.1(2)	C8-C7-C5	121.7(6)
O9-Ti1-Ti2	140.95(11)	O1-S1-C2	107.9(2)	C7-C8-C6	122.7(6)
O9-Ti1-O1	168.46(15)	Ti1-O1-Ti2	106.32(14)	O4-C9-C12	111.3(5)
O9-Ti1-O3	99.41(15)	C4-O1-Ti1	118.7(3)	O4-C9-C17	111.5(5)
O9-Ti1-O4	107.92(15)	C4-O1-Ti2	134.1(3)	C17-C9-C12	118.0(6)
O9-Ti1-O5	82.85(14)	C1-O2-Ti2 <sup>1</sup>	131.8(3)	O9-C10-C13	109.8(5)
O9-Ti1-O8	97.38(16)	C1-O3-Ti1	120.1(3)	O9-C10-C21	109.2(6)
O1-Ti2-Ti1	36.59(9)	Ti2-O4-Ti1	107.78(15)	C21-C10-C13	113.2(6)
O1-Ti2-O2 <sup>1</sup>	83.46(12)	C9-O4-Ti1	128.6(3)	O8-C11-C23	109.9(5)
O1-Ti2-O6	81.09(12)	C9-O4-Ti2	123.0(3)	O8-C11-C24	109.3(5)
O2 <sup>1</sup> -Ti2-Ti1	119.32(9)	S1-O5-Ti1	131.8(2)	C24-C11-C23	113.0(7)
O2 <sup>1</sup> -Ti2-O6	84.30(13)	S1-O6-Ti2	135.62(19)	O7-C14-C15	109.2(7)
O4-Ti2-Ti1	36.20(9)	C14-O7-Ti2	147.5(4)	C20-C14-O7	113.9(6)
O4-Ti2-O1	72.36(12)	C11-O8-Ti1	141.5(4)	C20-C14-C15	115.8(7)

O4-Ti2-O2 <sup>1</sup>	155.51(13)	C10-O9-Ti1	157.9(4)	O10-C16-C19	112.5(6)
O4-Ti2-O6	88.10(13)	C16-O10-Ti2	143.4(4)	O10-C16-C22	113.1(7)
O6-Ti2-Ti1	79.10(8)	O2-C1-O3	124.5(4)	C22-C16-C19	112.4(6)
O7-Ti2-Ti1	104.14(12)	O2-C1-C4	121.4(5)		

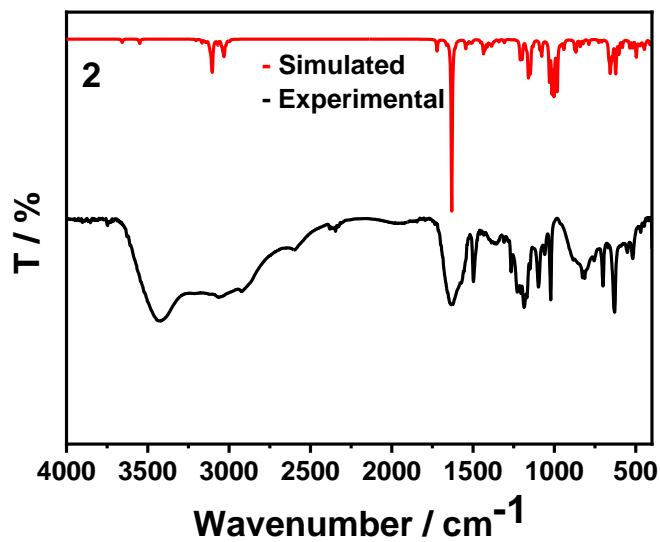
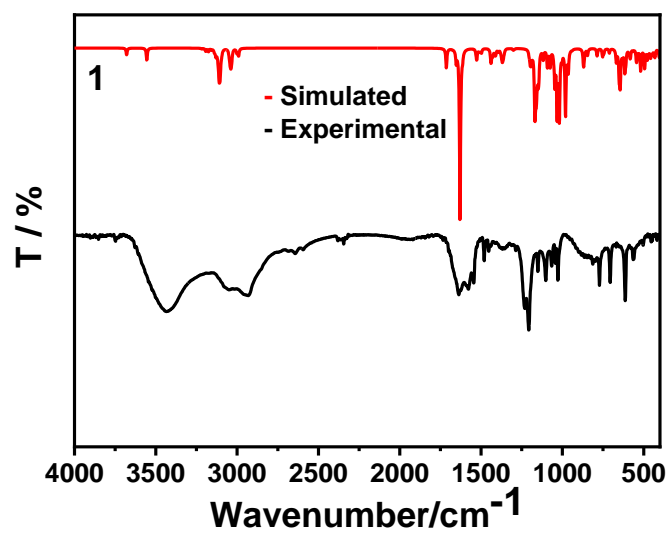


(a)

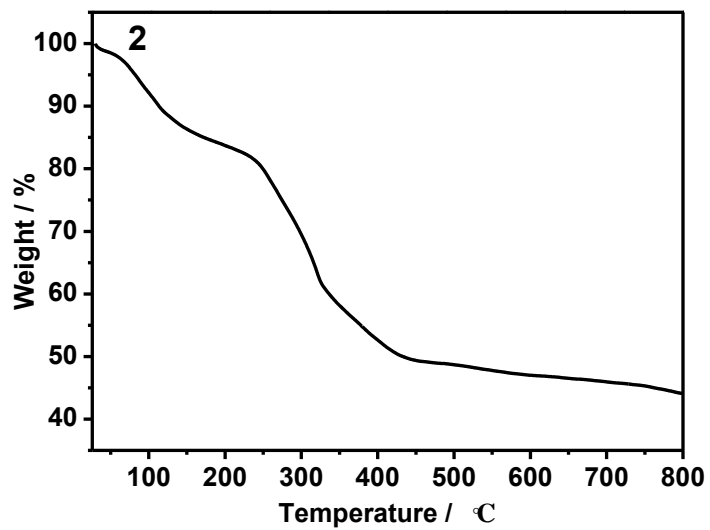
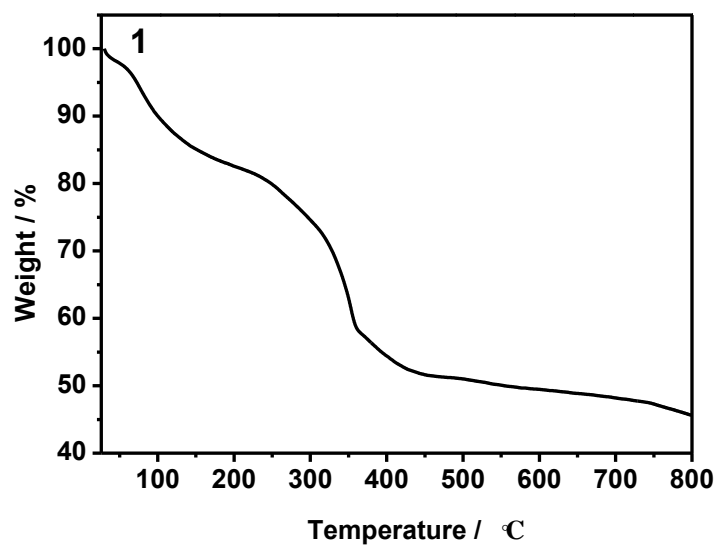


(b)

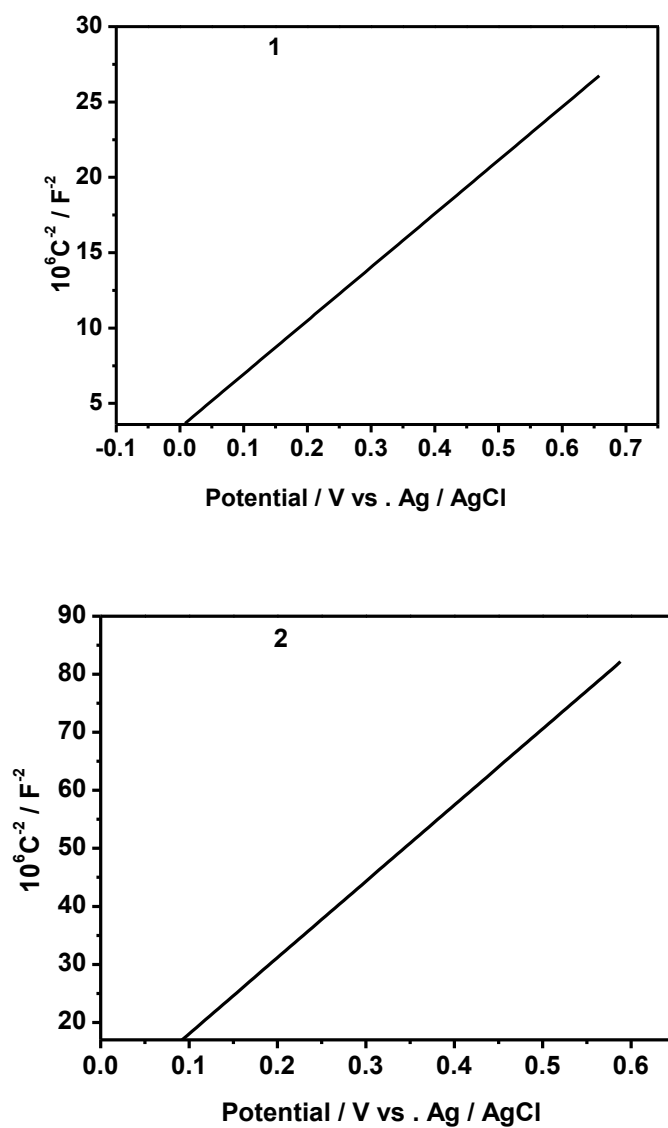
**Figure S1** Photos of the crystals **1** (a) and **2** (b).



**Figure S2** Comparison of Experimental and Computed (DFT/B3LYP method with 6-311G\* and lanl2dz basis set) FT-IR spectra of **1** and **2**.

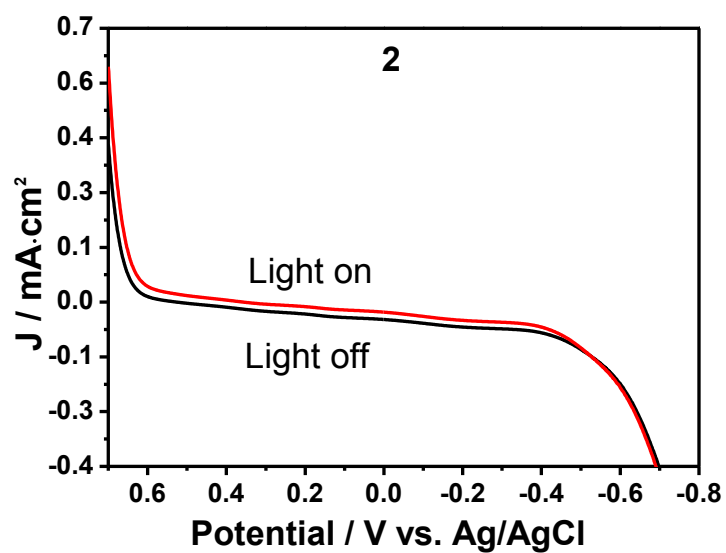
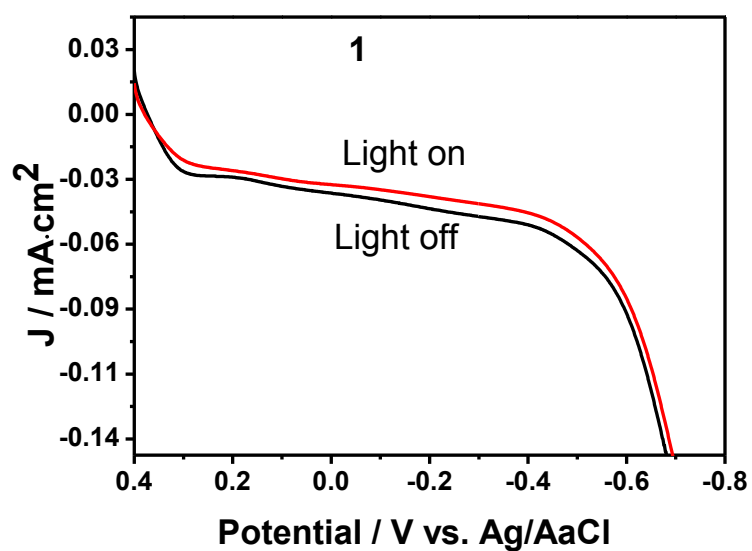


**Figure S3** TGA curves of **1** and **2**. All the two samples were treated by vacuum drying.

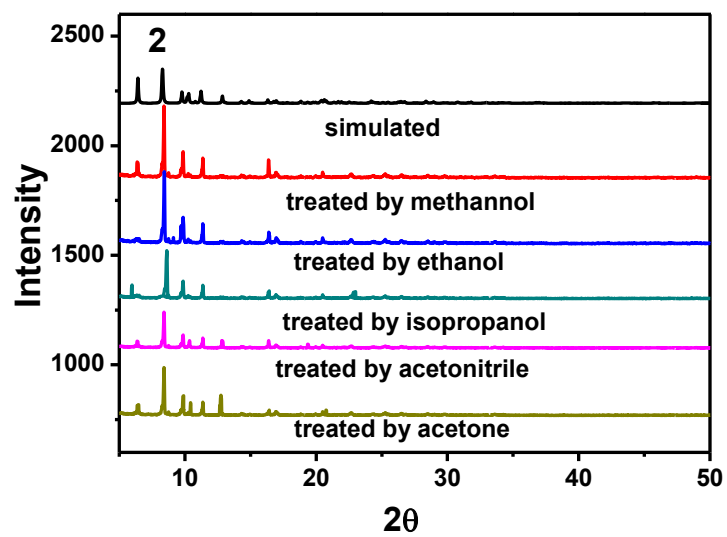
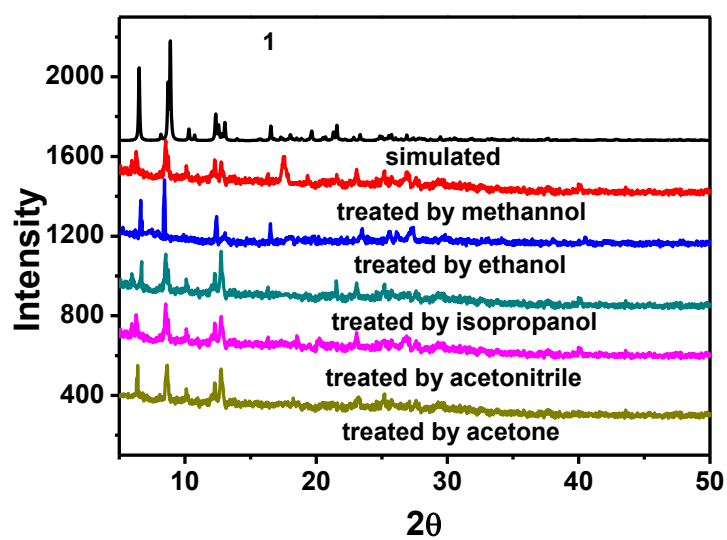


**Figure S4** Mott-Schottky plots for **1** and **2** in 0.1 M  $\text{Na}_2\text{SO}_4$  aqueous solution.

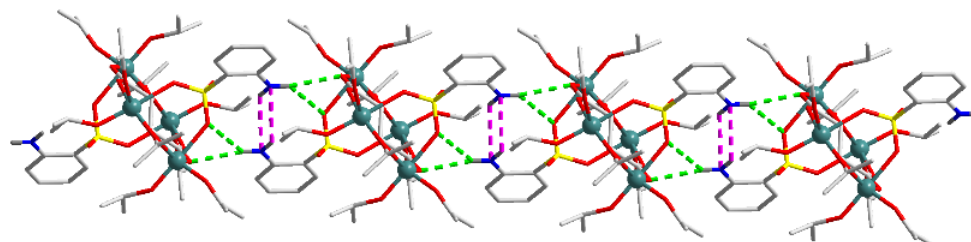




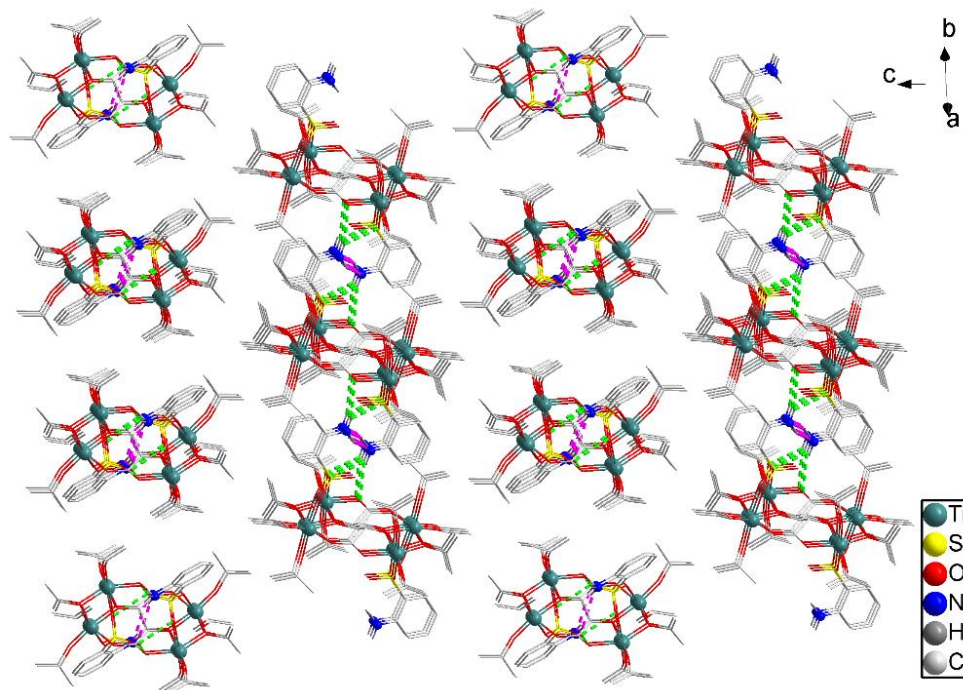
**Figure S5** Full range J-V curves of **1** and **2** in light-off (black) and light-on (red) conditions.



**Figure S6** XRD patterns of **1** and **2** under solvothermal treatment at room temperature for 24 h in different organic solvents.

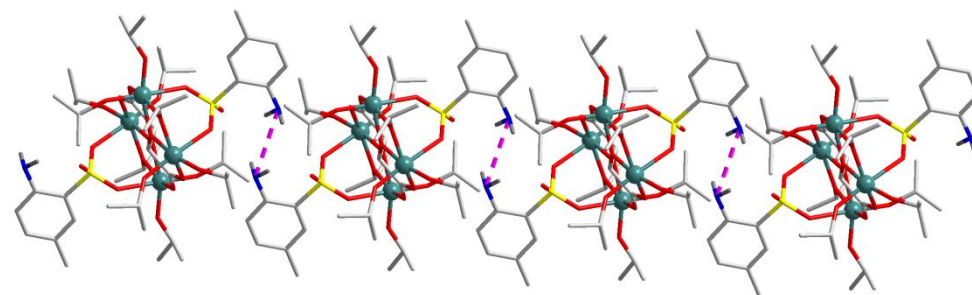


(a)

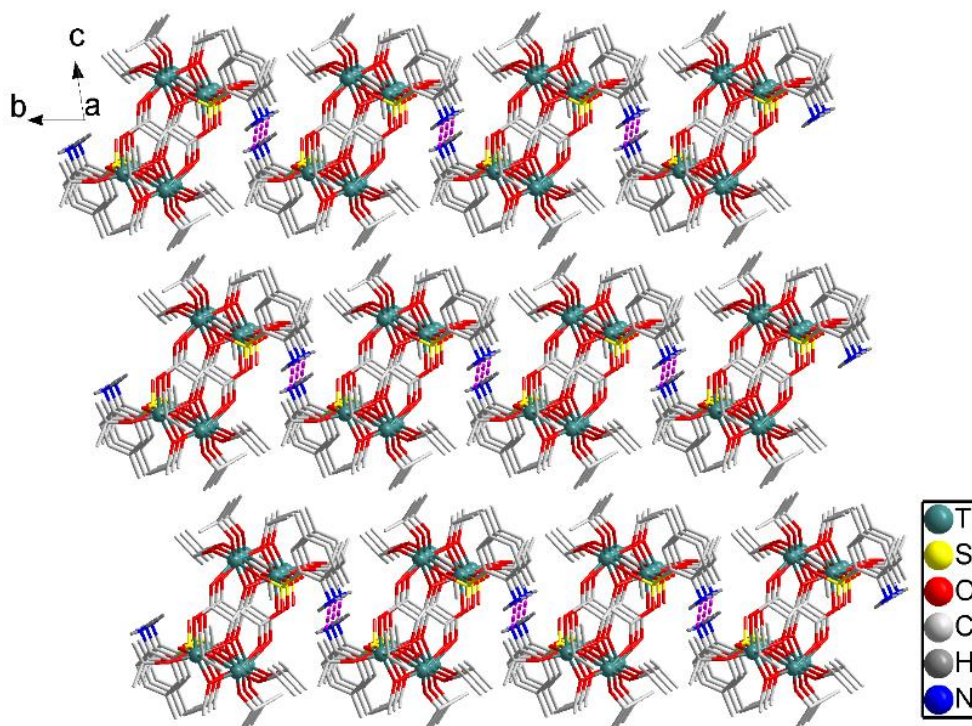


(b)

**Figure S7** (a) The hydrogen bonds between adjacent TOCs of **1**; (b) The 3D supramolecular network of **1**. The most hydrogen atoms are omitted for clarity.



(a)



(b)

**Figure S8** (a) The hydrogen bonds between adjacent TOCs of **2**; (b) The 3D supramolecular network of **2** viewing along *a*-axis. The most hydrogen atoms are omitted for clarity.