Electronic Supplementary Information

Reversible and irreversible stimuli-responsive chromism of a square-planar platinum(II) salt

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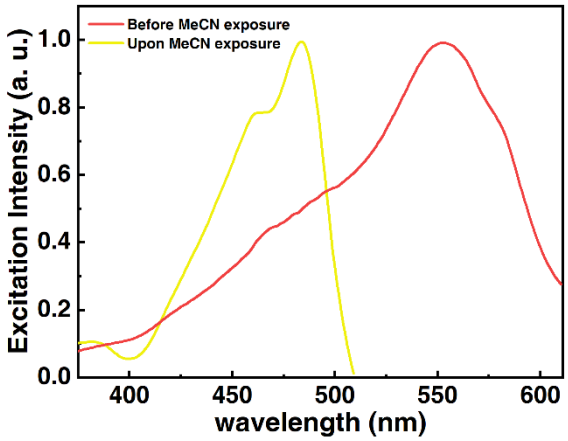

Fig. S1 Changes in excitation spectra before and after **1**OCN·OTf·H_2O contact with MeCN.

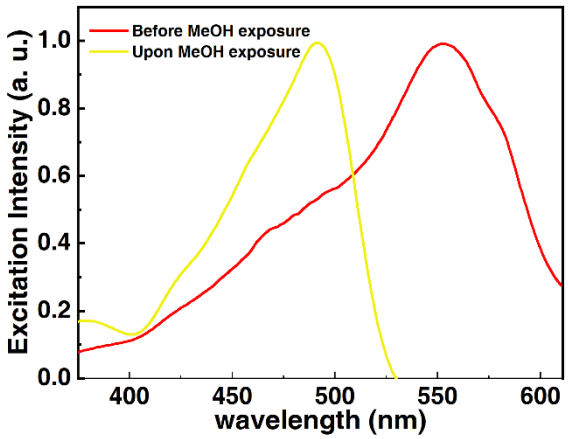

Fig. S2 Changes in excitation spectra before and after **1**OCN·OTf·H_2O contact with MeOH.

Table. S1 Colorimetric and photographs of **1**OCN·OTf·H_2O after contact with various organic chemical solutions

Organic chemical solvent	Colorimetric	Images
Acetonitrile	From red to yellow	
Methanol	From red to yellow	
Ethanol	Constant	
Carbon dichloride	Constant	
Carbon tetrachloride	Constant	
N-hexane	Constant	
Cyclohexane	Constant	
Acetone	Constant	
DMF	Dissolution	
DMSO	Dissolution	
THF	Constant	
Petroleum ether	Constant	
Ethyl ether	Constant	
Ethyl acetate	Constant	
Acetaldehyde	Constant	
Formaldehyde	Constant	
Butyl cyanide	Constant	
N-Butyronitrile	Constant	

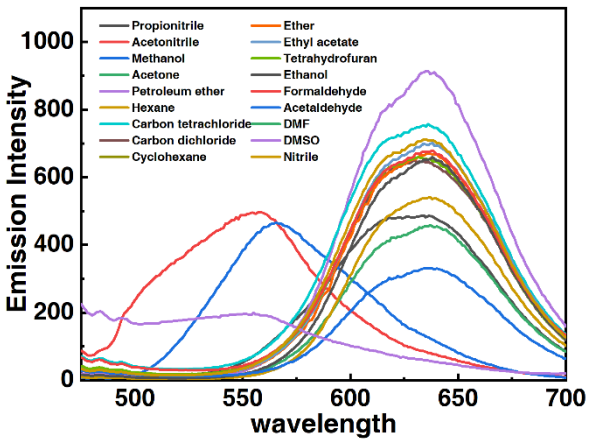

Fig. S3 Emission selectivity of **1**OCN·OTf·H_2O to MeCN.

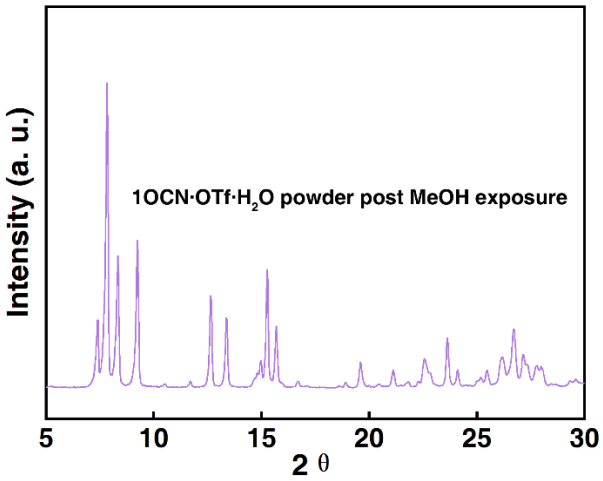

Fig. S4 XRD pattern of **1**OCN·OTf·H_2O upon MeOH exposure.

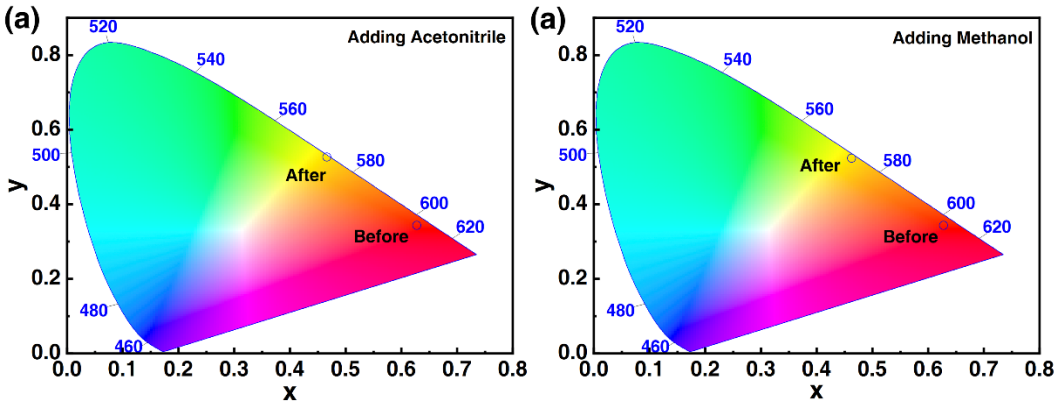

Fig. S5 (a) **1**OCN·OTf·H_2O phosphorescence CIE diagram before and after contact with MeCN, (b) **1**OCN·OTf·H_2O phosphorescence CIE diagram before and after contact with MeOH.

Table. S2: Crystal data and structure refinement for [Pt(tpy)OCN]·OTf·H_2O.

Compound	[Pt(tpy)OCN]·OTf·H_2O
Empirical formula	$C_{17}H_{12}F_3N_4O_{4.5}PtS$
Formula weight	628.46
Temperature/K	292.99(11)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.78310(10)
b/Å	23.8581(3)
c/Å	23.5997(3)
α/°	90
β/°	91.6080(10)
γ/°	90
Volume/Å^3	3817.68(9)
Z	8
ρ_{calc}g/cm^3	2.187
μ/mm^{-1}	15.394
F(000)	2392.0
Crystal size/mm^3	0.13 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.268 to 143.418
Index ranges	$-6 \le h \le 8$, $-27 \le k \le 29$, $-28 \le l \le 28$
Reflections collected	21395
Independent reflections	7263 [R_{int} = 0.0413, R_{sigma} = 0.0401]
Data/restraints/parameters	7263/0/553
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0364, wR_2 = 0.1038
Final R indexes [all data]	R_1 = 0.0406, wR_2 = 0.1063
Largest diff. peak/hole / e Å^{-3}	0.71/-0.88

The obtained single crystals have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number: [Pt(tpy)OCN]·OTf·H_2O (2263879).

Table. S3: Crystal data and structure refinement for [Pt(tpy)OCN]·OTf.

Compound	[Pt(tpy)OCN]·OTf
Empirical formula	$C_{17}H_{11}F_3N_4O_4PtS$
Formula weight	619.45
Temperature/K	199.98(10)
Crystal system	monoclinic
Space group	Cc
a/Å	13.9994(10)
b/Å	19.0666(15)
c/Å	6.7719(5)
α/°	90
β/°	95.207(7)
γ/°	90
Volume/Å^3	1800.1(2)
Z	4
ρ_{calc}g/cm^3	2.286
μ/mm^{-1}	16.290
F(000)	1176.0
Crystal size/mm^3	0.14 × 0.12 × 0.09
Radiation	Cu Kα (λ = 1.54178)
2Θ range for data collection/°	7.856 to 143.866
Index ranges	$-17 \leq h \leq 17$, $-23 \leq k \leq 22$, $-8 \leq l \leq 7$
Reflections collected	4075
Independent reflections	2008 [R_{int} = 0.0331, R_{sigma} = 0.0311]
Data/restraints/parameters	2008/206/272
Goodness-of-fit on F^2	1.156
Final R indexes [I>=2σ (I)]	R_1 = 0.0332, wR_2 = 0.0872
Final R indexes [all data]	R_1 = 0.0341, wR_2 = 0.0873
Largest diff. peak/hole / e Å^{-3}	1.19/-1.54
Flack parameter	0.477(15)

The obtained single crystals have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number: [Pt(tpy)OCN]·OTf (2263889).

Experimental

Single crystals of $C_{17}H_{11}F_3N_4O_4PtS$were [Pt(tpy)OCN]·OTf. A suitable crystal was selected and [Pt(tpy)OCN]·OTf on a multiwire proportional diffractometer. The crystal was kept at 199.98(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. **42**, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. **A71**, 3-8.

3. Sheldrick, G.M. (2015). Acta Cryst. **C71**, 3-8.