Electronic Supplementary Information

Acid- and base-stable porous mechanically interlocked 2D metal-organic polyrotaxane for in situ organochlorine insecticide encapsulation, sensing and removing

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Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{40}H_{26}N_4O_{12}S_2Zn_2$
Formula weight	949.51
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.7927(10)
b/Å	12.7479(11)
c/Å	17.1763(16)
α/°	103.520(4)
β/°	105.261(4)
γ/°	97.511(4)
Volume/Å^3	2370.6(4)
Z	2
ρ_{calc}g/cm^3	1.330
μ/mm^{-1}	1.158
F(000)	964
Crystal size/mm^3	0.080 × 0.020 × 0.020
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.358 to 45.138
Index ranges	$-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $-18 \leq l \leq 18$
Reflections collected	27819
Independent reflections	6220 [R_{int} = 0.0851, R_{sigma} = 0.0920]
Data/restraints/parameters	6220/0/541
Goodness-of-fit on F^2	1.000
Final R indexes [I>=2σ (I)]	R_1 = 0.0445, wR_2 = 0.0942
Final R indexes [all data]	R_1 = 0.0952, wR_2 = 0.1096
Largest diff. peak/hole / e Å^{-3}	0.31/-0.34

Note on the structure refinement:

The pyridyl group with N3 can rotate or oscillate around the Zn2-N3 and C37-C40 bond. The same is possible for the pyridyl group with N1 around Zn1-N1 and C31-C34. Such a disorder would induce larger displacement parameters for the N3(N1)-bonded carbon atoms C35(C29) and C39(C33) than for the N3(N1) atom itself which is bonded to Zn. Thereby larger differences in the anisotropic displacement parameters along the N-C chemical bonds will lead to a failure in the Hirshfeld test.

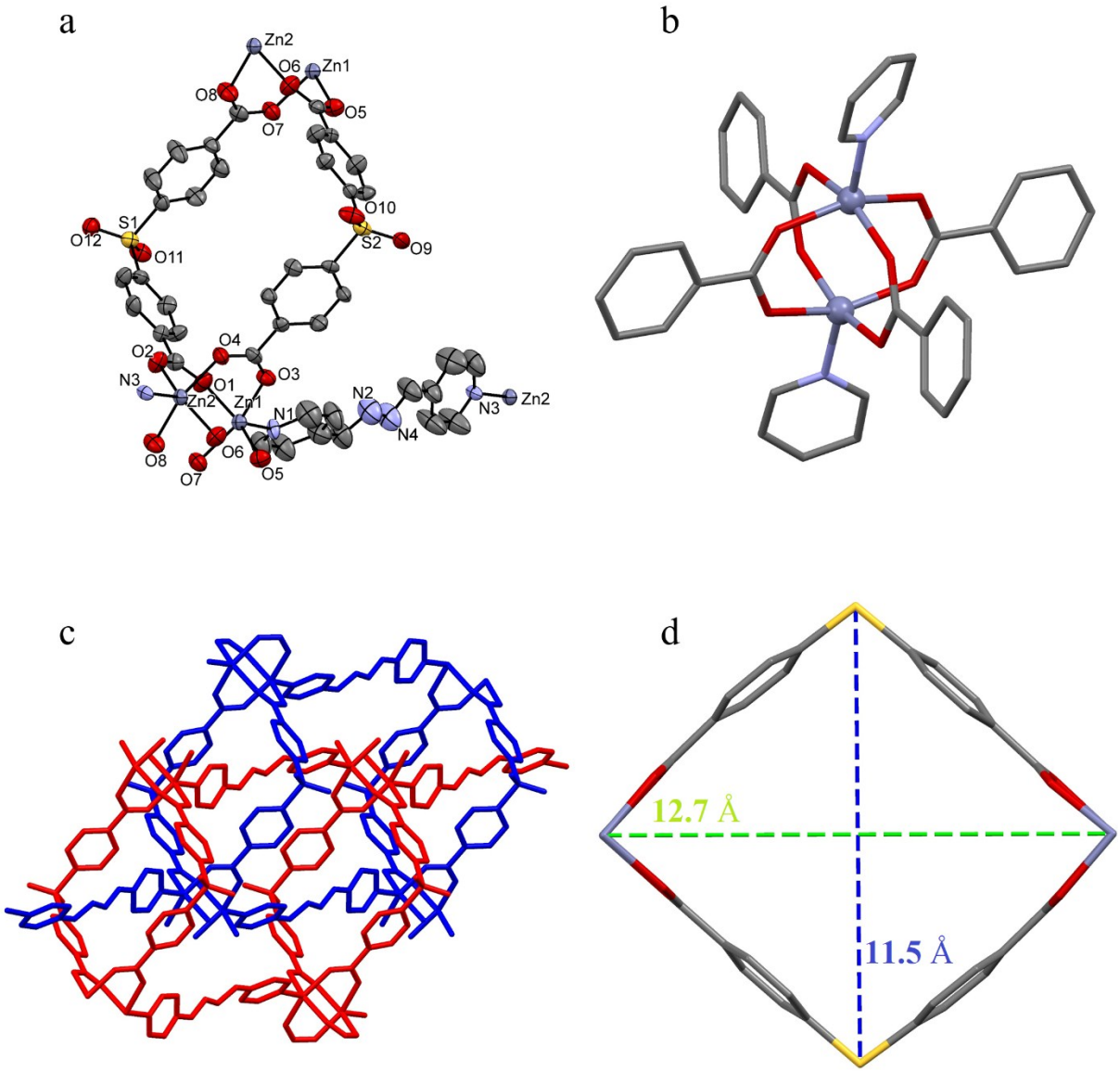

Fig. S1. a) Ortep diagram of **1** along c axis (hydrogen atoms omitted), b) Paddle wheel zinc building unit (only 6-membered rings remained), c) Double entanglement to make an interlocked metal-organic polyrotaxane (c axis view) and d) The rectangular ring with the representation of window size.

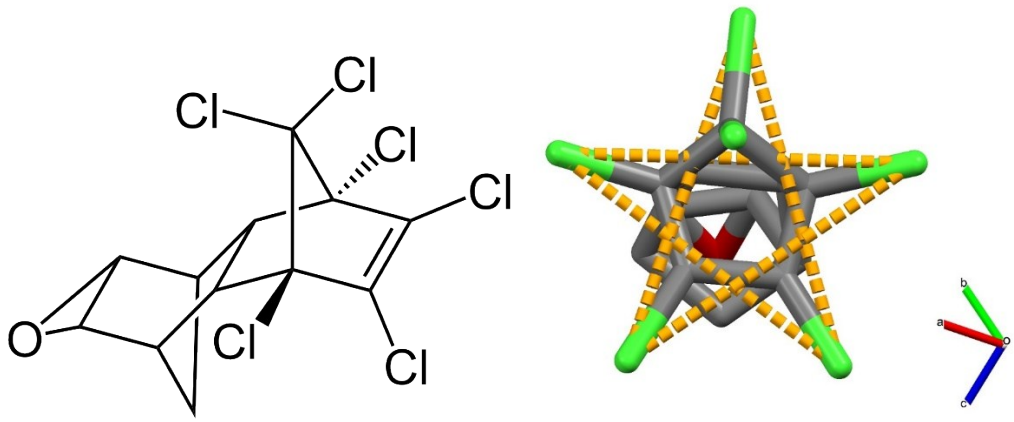

Fig. S2 Dieldrin Lewis structure (left) and star-like view (right)

Table S2

Calculated and founded CHN elemental analysis for **1** and dieldrin@**1**

Element (%) / Compound	C	H	N
Calculated **1**	50.60	2.76	5.90
Found **1**	51.05	3.23	6.09
Found dieldrin@**1**	48.84	2.29	5.69

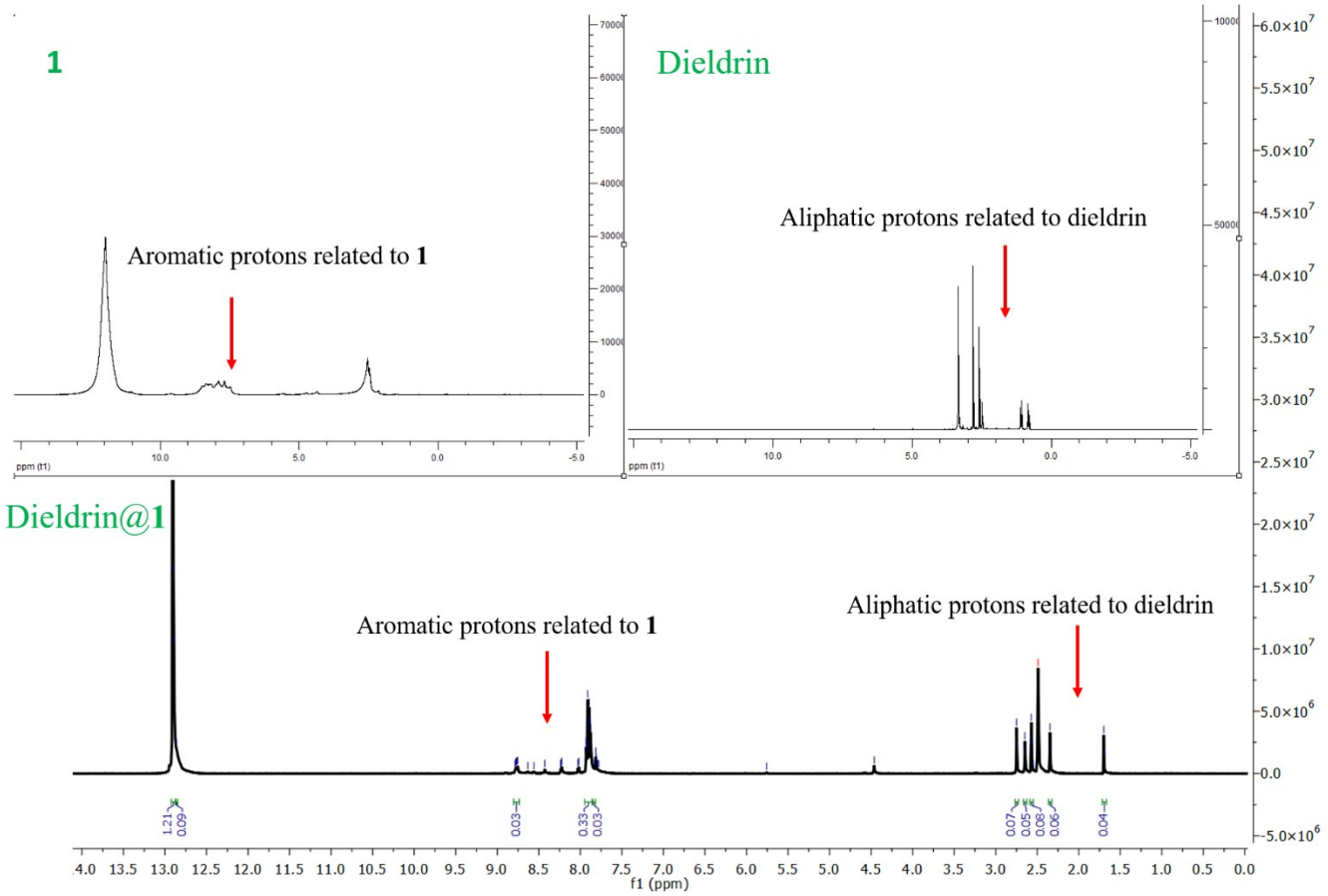

Fig. S3. ^{1}H NMR spectrum of **1** (up, left), dieldrin (up, right) and dieldrin@**1** (bottom) in DMSO-d_6 digested in 100 µL of D_2SO_4.

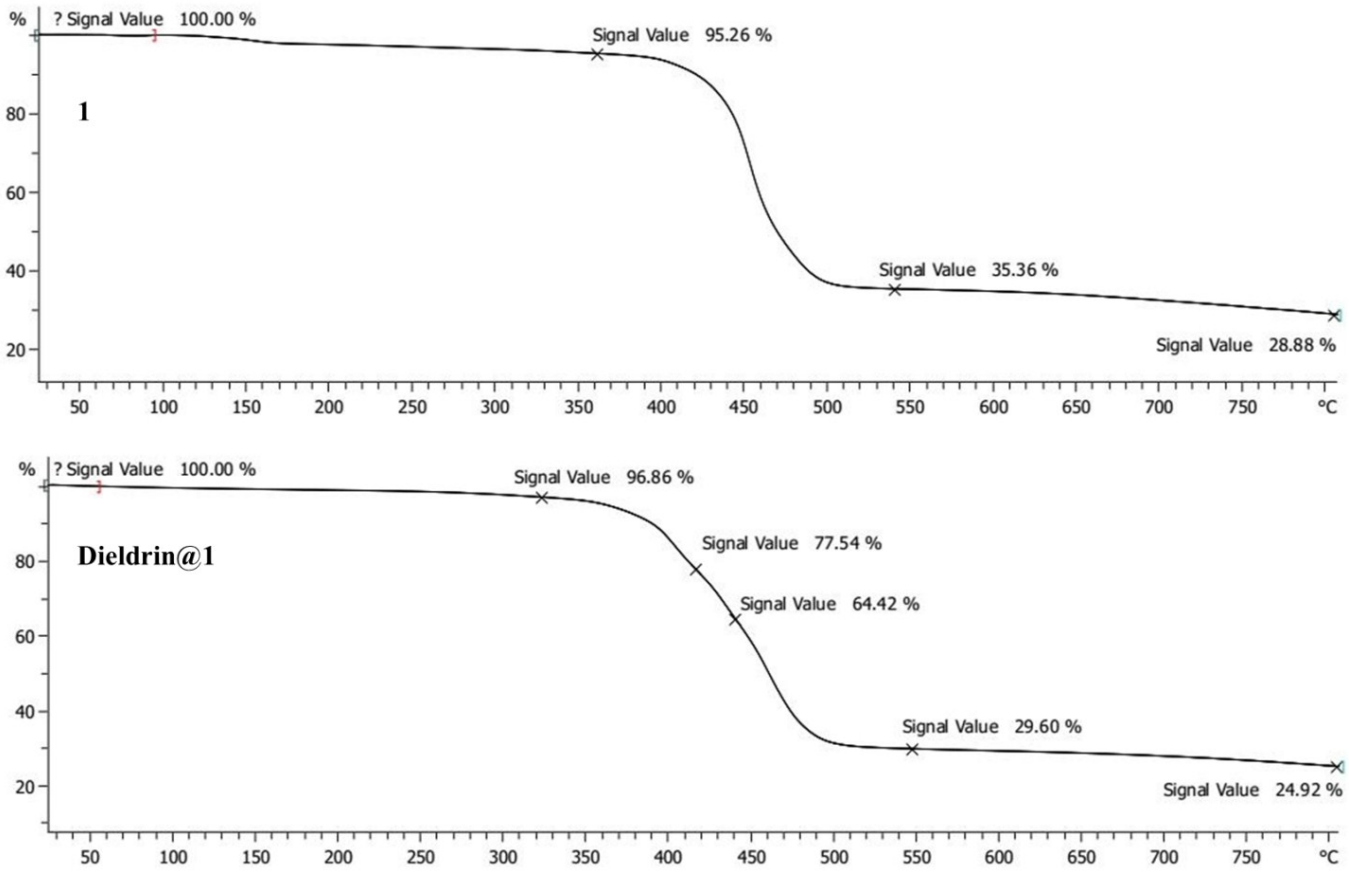

Fig. S4. TGA curve of **1** and dieldrin@**1.**

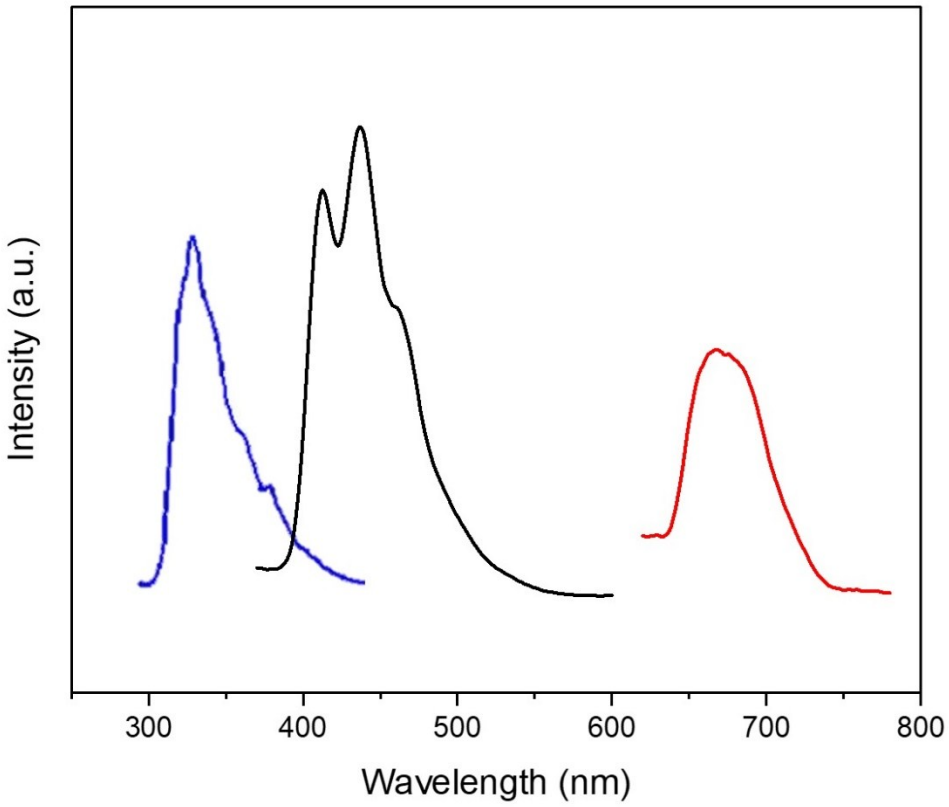

Fig. S5 The emission spectrum of compound **1** (black), H_2sdba (blue) and 4-bpdb (red) at room temperature upon excitation at 331, 329 and 523 nm respectively.

Note: crystallographic data in CIF available in *CCDC 1825208*.