Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

A fast and highly selective Congo red adsorption material based on cadmium-phosphonate network

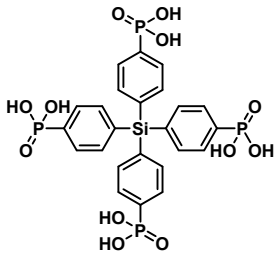
Jing Ai,[a, b] Hong-Rui Tian,[b] Xue Min*[c], Zi-Chuan Wang,*[a] and Zhong-Ming Sun *[a, b]

***a.** School of Materials Science and Engineering & National Institute for Advanced Materials, Tianjin Key Lab for Rare Earth Materials and Applications, Center for Rare Earth and Inorganic Functional Materials, State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300350, China*

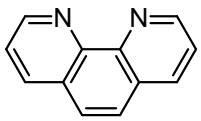
E-mail:sunlab@nankai.edu.cn, zcwang@nankai.edu.cn; Web: http://zhongmingsun.weebly.com

***b.** State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 5625 Renmin Street, Changchun, Jilin 130022, China*

***c.** School of Chemistry and Chemical Engineering, Wuhan Textile University, Wuhan 430200, China*
E-mail: xmin@wtu.edu.cn

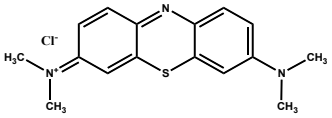


(H_8L)

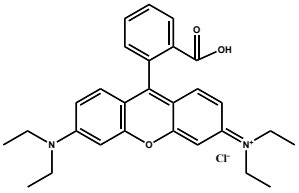


(phen)

Scheme S1. Chemical structure of ligand H_8L and phen.



Methylene Blue (MB)



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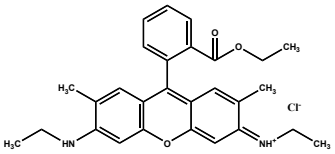
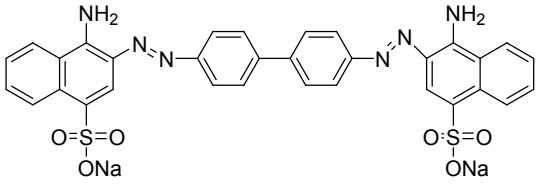


Rhodamine 6G (R6G)



Congo red (CR)

Scheme S2. Chemical structures of organic dyes used in this work.

Table S1. Crystallographic data for compound **1**.

compound	**1**
Formula	$Cd_4Si_2P_8C_{96}N_8O_{28}H_{48}$
F_w	2515.05
Crystal system	triclinic
Space group	*P*-1
a /Å	14.0172(1)
b / Å	14.5930(1)
c / Å	25.8504(2)
α / °	105.4310(1)
B / °	95.932(2)
γ / °	100.167(2)
V, Å^3	4953.8(6)
Z	2
D_c, mg/mm^3	1.704
μ, mm^{-1}	1.083
reflection collected	31606
GOF on F^2	1.076

R_1/wR_2 ($I > 2\sigma(I)$)	0.0619 / 0.1392
R_1/wR_2 (all data)	0.0881 / 0.1569

Table S2. Selected bond lengths for **1**.

Cd(1)-O(7)	2.288(5)	Cd(3)-O(11)#5	2.216(4)
Cd(1)-O(21)#1	2.278(4)	Cd(3)-O(12)	2.350(4)
Cd(1)-O(23)	2.438(4)	Cd(3)-O(13)	2.194(4)
Cd(1)-O(28)#2	2.207(4)	Cd(3)-O(14)	2.410(4)
Cd(1)-N(1)	2.345(5)	Cd(3)-N(5)	2.307(5)
Cd(1)-N(2)	2.315(5)	Cd(3)-N(6)	2.347(5)
Cd(2)-O(18)#2	2.256(4)	Cd(4)-O(1)	2.222(7)
Cd(2)-O(22)	2.190(5)	Cd(4)-O(4)	2.357(5)
Cd(2)-O(24)#3	2.279(4)	Cd(4)-O(5)#5	2.223(4)
Cd(2)-O(26)#4	2.418(4)	Cd(4)-O(6)	2.348(5)
Cd(2)-N(7)	2.363(6)	Cd(4)-N(3)	2.350(7)
Cd(2)-N(8)	2.357(6)	Cd(4)-N(4)	2.356(6)

Symmetry code: #1 1+X, +Y, +Z; #2 1-X, 2-Y,1-Z; #3 -X, 2-Y, -Z; #4 -X, 2-Y, 1-Z; #5 +X, -1+Y, +Z.

Table S3. Selected bond angles for **1**.

O(7)-Cd(1)-O(23)	78.74(17)	O(11)#5-Cd(3)-O(12)	91.94(16)
O(7)-Cd(1)-N(1)	111.4(2)	O(11)#5-Cd(3)-O(14)	93.28(15)
O(7)- Cd(1)-N(2)	165.68(18)	O(11)#5-Cd(3)-N(5)	96.77(17)
O(21)#1-Cd(1)-O(7)	83.00(18)	O(11)#5-Cd(3)-N(6)	166.61(16)
O(21)#1-Cd(1)-O(23)	160.74(15)	O(12)-Cd(3)-O(14)	162.60(15)
O(21)#1-Cd(1)-N(1)	97.76(16)	O(13)-Cd(3)-O(11)#5	106.16(16)
O(21)#1-Cd(1)-N(2)	82.72(17)	O(13)- Cd(3)-O(12)	78.05(15)
O(28)#2-Cd(1)-O(7)	92.5(2)	O(13)-Cd(3)-O(14)	84.56(15)
O(28)#2-Cd(1)-O(21)#1	90.12(15)	O(13)-Cd(3)-N(5)	153.96(17)
O(28)#2-Cd(1)-O(23)	96.71(15)	O(13)-Cd(3)-N(6)	86.60(16)
O(28)#2-Cd(1)-N(1)	155.55(18)	N(5)-Cd(3)-O(12)	89.21(17)
N(1)- Cd(1)-N(2)	86.51(17)	N(5)-Cd(3)-O(14)	106.61(16)
N(2)- Cd(1)-O (23)	83.37(16)	N(5)-Cd(3)-N(6)	71.76(17)
N(2)- Cd(1)-O (23)	115.57(16)	N(6)-Cd(3)-O(12)	94.72(16)
O(18)#2-Cd(1)-N (1)	71.70(19)	N(6)-Cd(3)-O(14)	83.77(15)
O(18)#2-Cd(2)-O(24)#3	81.32(14)	O(1) Cd(4)-O(4)	90.8(3)
O(18)#2-Cd(2)-O(26)#4	86.33(15)	O(1)-Cd(4)-O(5)#5	105.28(18)
O(18)#2-Cd(2)-N(7)	157.63(19)	O(1)-Cd(4)-O(6)	95.2(2)
O(22)-Cd(2)-N 8)	87.37(19)	O(1)-Cd(4)-N(3)	157.8(2)
O(22)-Cd(2)-O(18)#2	103.29(19)	O(1)-Cd(4)-N(4)	87.0(2)
O(22)-Cd(2)-O(24)#3	91.61(16)	O(5)#5-Cd(4)-O(4)	88.06(17)
O(22)-Cd(2)-(26)#4	84.11(16)	O(5)#5-Cd(4)-O(6)	86.03(16)
O(22)-Cd(2)-N(7)	98.8(2)	O(5)#5-Cd(4)-N(3)	96.42(18)

O(22)-Cd(2)-N(8)	168.9(2)	O(5)#5-Cd(4)-N(4)	166.8(2)
O(24)#3-Cd(2)-O(26)#4	165.64(14)	O(6)-Cd(4)-O(4)	172.6(2)
O(24)#3-Cd(2)-N(7)	101.48(16)	O(6)-Cd(4)-N(3)	81.3(2)
O(24)#3-Cd(2)-N(8)	92.90(16)	O(6)-Cd(4)-N(4)	88.17(19)
N(7)-Cd(2)-(26)#4	92.73(17)	N(3)-Cd(4)-O(4)	94.9(2)
N(8)-Cd(2)-O(26)#4	93.82(16)	N(3)-Cd(4)-N(4)	71.0(2)
N(8) Cd(2)-N(7)	70.4(2)	N(4)-Cd(4)-O(4)	96.66(19)

Symmetry code: #1 1+X, +Y, +Z; #2 1-X, 2-Y,1-Z; #3 -X, 2-Y, -Z; #4 -X, 2-Y, 1-Z; #5 +X, -1+Y, +Z.

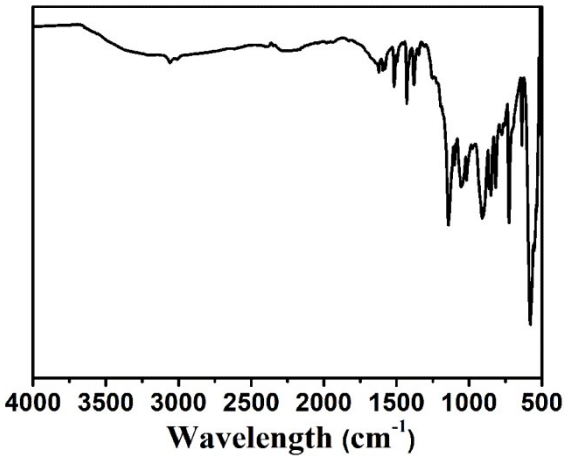


Fig. S1. Infrafred spectra of compound **1**.

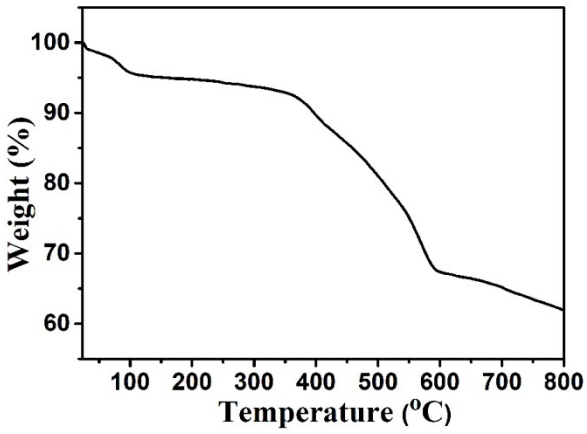


Fig. S2. Thermogravimetric analysis data for compound **1**.

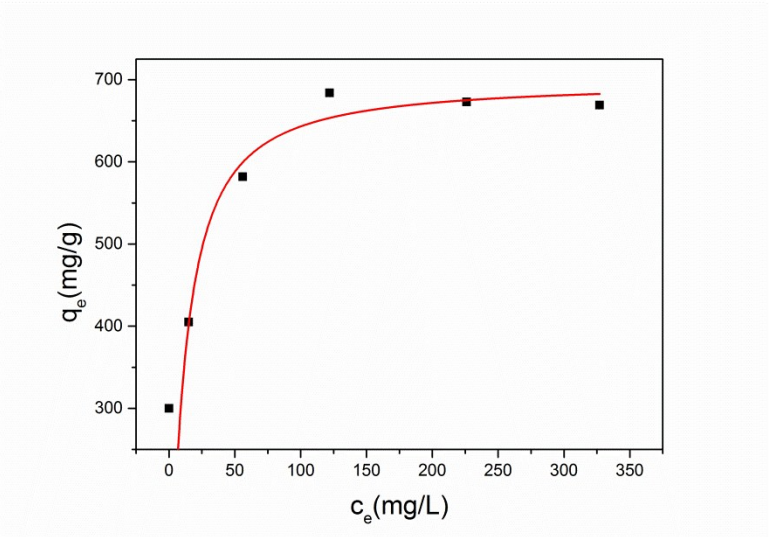


Fig. S3. Adsorption isothermal of CR on the compound **1**.

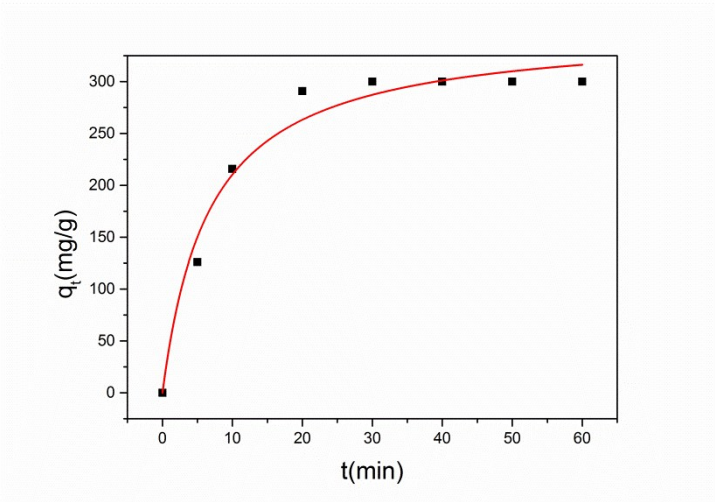


Fig. S4. The U adsorption capacity under different contact times on the compound **1**.