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Supplementary Information

A microporous Cd-MOF based on a hexavalent silicon-centred connector and luminescent sensing of small molecules

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Table S1 Selected bonds and angles for 1

Cd(1)-O(8)#1	2.216(3)	O(8)#1-Cd(1)-O(9)#2	112.99(10)
Cd(1)-O(9)#2	2.251(3)	O(8)#1-Cd(1)-O(2W)	94.53(12)
Cd(1)-O(2W)	2.276(3)	O(9)#2-Cd(1)-O(2W)	81.98(11)
Cd(1)-O(3W)	2.339(3)	O(8)#1-Cd(1)-O(3W)	88.26(10)
Cd(1)-O(12)	2.339(3)	O(9)#2-Cd(1)-O(3W)	82.32(10)
Cd(1)-O(11)	2.354(3)	O(2W)-Cd(1)-O(3W)	163.88(11)
Cd(1)-C(25)	2.694(4)	O(8)#1-Cd(1)-O(12)	150.04(9)
Cd(2)-O(4)#3	2.230(3)	O(9)#2-Cd(1)-O(12)	95.58(10)
Cd(2)-O(5W)	2.249(3)	O(2W)-Cd(1)-O(12)	98.36(13)
Cd(2)-O(10)#4	2.258(3)	O(3W)-Cd(1)-O(12)	86.76(10)
Cd(2)-O(7)	2.313(3)	O(8)#1-Cd(1)-O(11)	97.81(10)
Cd(2)-O(4W)	2.365(3)	O(9)#2-Cd(1)-O(11)	148.53(11)
Cd(2)-O(8)	2.446(3)	O(2W)-Cd(1)-O(11)	89.60(11)
Cd(2)-C(17)	2.737(4)	O(3W)-Cd(1)-O(11)	105.77(10)
Cd(3)-O(3)#5	2.249(3)	O(12)-Cd(1)-O(11)	55.57(9)
Cd(3)-O(1)#6	2.285(3)	O(8)#1-Cd(1)-C(25)	124.73(10)
Cd(3)-O(1W)	2.286(3)	O(9)#2-Cd(1)-C(25)	122.27(11)
Cd(3)-O(5)	2.291(3)	O(2W)-Cd(1)-C(25)	93.99(12)
Cd(3)-O(6)	2.381(3)	O(3W)-Cd(1)-C(25)	97.45(11)
Cd(3)-O(2)#6	2.388(3)	O(12)-Cd(1)-C(25)	27.72(10)
Cd(3)-C(16)	2.683(4)	O(11)-Cd(1)-C(25)	27.86(10)
Cd(3)-C(9)#6\	2.692(4)	O(4)#3-Cd(2)-O(5W)	96.35(11)
O(1)-Cd(3)#7	2.285(3)	O(4)#3-Cd(2)-O(10)#4	100.06(11)
O(2)-Cd(3)#7	2.388(3)	O(5W)-Cd(2)-O(10)#4	156.98(13)
O(3)-Cd(3)#2	2.249(3)	O(4)#3-Cd(2)-O(7)	111.36(10)
O(4)-Cd(2)#3	2.230(3)	O(5W)-Cd(2)-O(7)	100.60(11)
O(8)-Cd(1)#1	2.216(3)	O(10)#4-Cd(2)-O(7)	88.35(11)
O(9)-Cd(1)#5	2.251(3)	O(4)#3-Cd(2)-O(4W)	86.64(12)
O(10)-Cd(2)#4	2.258(3)	O(5W)-Cd(2)-O(4W)	84.30(13)
C(9)-Cd(3)#7	2.692(4)	O(10)#4-Cd(2)-O(4W)	80.69(12)
C(4)-C(9)-Cd(3)#7	171.8(3)	O(7)-Cd(2)-O(4W)	160.43(12)
O(6)-C(16)-Cd(3)	62.5(2)	O(4)#3-Cd(2)-O(8)	165.69(10)
O(5)-C(16)-Cd(3)	58.5(2)	O(5W)-Cd(2)-O(8)	83.08(10)
C(12)-C(16)-Cd(3)	178.3(3)	O(10)#4-Cd(2)-O(8)	84.90(10)
O(7)-C(17)-Cd(2)	57.22(19)	O(7)-Cd(2)-O(8)	55.04(9)
O(8)-C(17)-Cd(2)	63.33(18)	O(4W)-Cd(2)-O(8)	107.48(11)
C(14)-C(17)-Cd(2)	176.6(3)	O(4)#3-Cd(2)-C(17)	138.42(11)
O(12)-C(25)-Cd(1)	60.17(19)	O(5W)-Cd(2)-C(17)	93.33(11)

O(11)-C(25)-Cd(1)	60.86(19)	O(10)#4-Cd(2)-C(17)	85.03(11)
C(22)-C(25)-Cd(1)	177.2(3)	O(7)-Cd(2)-C(17)	27.09(11)
C(16)-O(5)-Cd(3)	93.3(2)	O(4W)-Cd(2)-C(17)	134.63(13)
C(16)-O(6)-Cd(3)	89.8(2)	O(3)#5-Cd(3)-O(1)#6	96.91(11)
C(17)-O(7)-Cd(2)	95.7(2)	O(3)#5-Cd(3)-O(1W)	91.74(11)
C(17)-O(8)-Cd(2)	88.7(2)	O(1)#6-Cd(3)-O(1W)	115.63(13)
O(8)-Cd(2)-C(17)	28.00(10)	O(3)#5-Cd(3)-O(5)	109.60(11)
O(5)-Cd(3)-O(6)	55.81(10)	O(1)#6-Cd(3)-O(5)	104.26(13)
O(5)-Cd(3)-C(16)	28.21(11)	O(1W)-Cd(3)-O(5)	131.91(11)
O(6)-Cd(3)-C(16)	27.60(11)	O(3)#5-Cd(3)-O(6)	83.71(12)
O(8)#1-Cd(1)-O(12)	158.25(14)	O(1W)-Cd(3)-O(6)	86.03(12)
C(17)-O(8)-Cd(1)#1	127.3(2)	O(3)#5-Cd(3)-O(2)#6	144.37(11)
Cd(1)#1-O(8)-Cd(2)	105.42(10)	O(1)#6-Cd(3)-O(2)#6	55.14(10)
C(24)-O(9)-Cd(1)#5	118.5(3)	O(1W)-Cd(3)-O(2)#6	83.40(12)
C(24)-O(10)-Cd(2)#4	141.0(3)	O(5)-Cd(3)-O(2)#6	99.49(12)
C(25)-O(11)-Cd(1)	91.3(2)	O(6)-Cd(3)-O(2)#6	130.77(12)
C(25)-O(12)-Cd(1)	92.1(2)	O(3)#5-Cd(3)-C(16)	96.95(11)
O(1)-C(9)-Cd(3)#7	57.8(2)	O(1)#6-Cd(3)-C(16)	131.91(14)
O(2)-C(9)-Cd(3)#7	62.5(2)	O(1W)-Cd(3)-C(16)	109.70(12)
O(2)#6-Cd(3)-C(9)#6	27.71(11)	O(2)#6-Cd(3)-C(16)	117.97(12)
C(16)-Cd(3)-C(9)#6	131.50(12)	O(3)#5-Cd(3)-C(9)#6	120.88(11)
C(9)-O(1)-Cd(3)#7	94.7(3)	O(1)#6-Cd(3)-C(9)#6	27.52(11)
C(9)-O(2)-Cd(3)#7	89.8(2)	O(1W)-Cd(3)-C(9)#6	99.05(13)
C(8)-O(3)-Cd(3)#2	119.0(2)	O(5)-Cd(3)-C(9)#6	105.07(11)
C(8)-O(4)-Cd(2)#3	127.6(2)	O(6)-Cd(3)-C(9)#6	154.44(12)

Symmetry codes: #1-x+1,-y,-z+1; #2 x-1,y,z; #3 -x+2,-y,-z+2; #4-x+2,-y,-z+1; #5 x+1,y,z; #6 x+1/2,-y+1/2,z+1/2; #7 x-1/2,-y+1/2,z-1/2

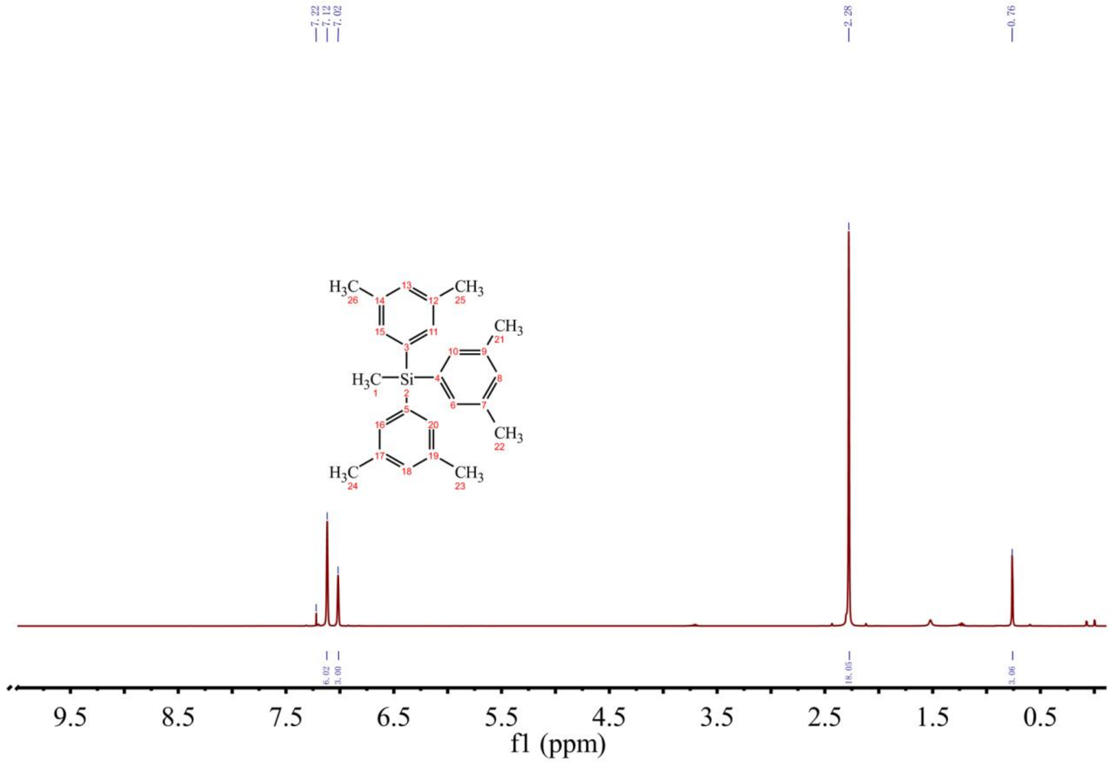

Figure S1 The ^{1}H-NMR spectrum of tris(3,5-dimethylphenyl)(methyl)silane

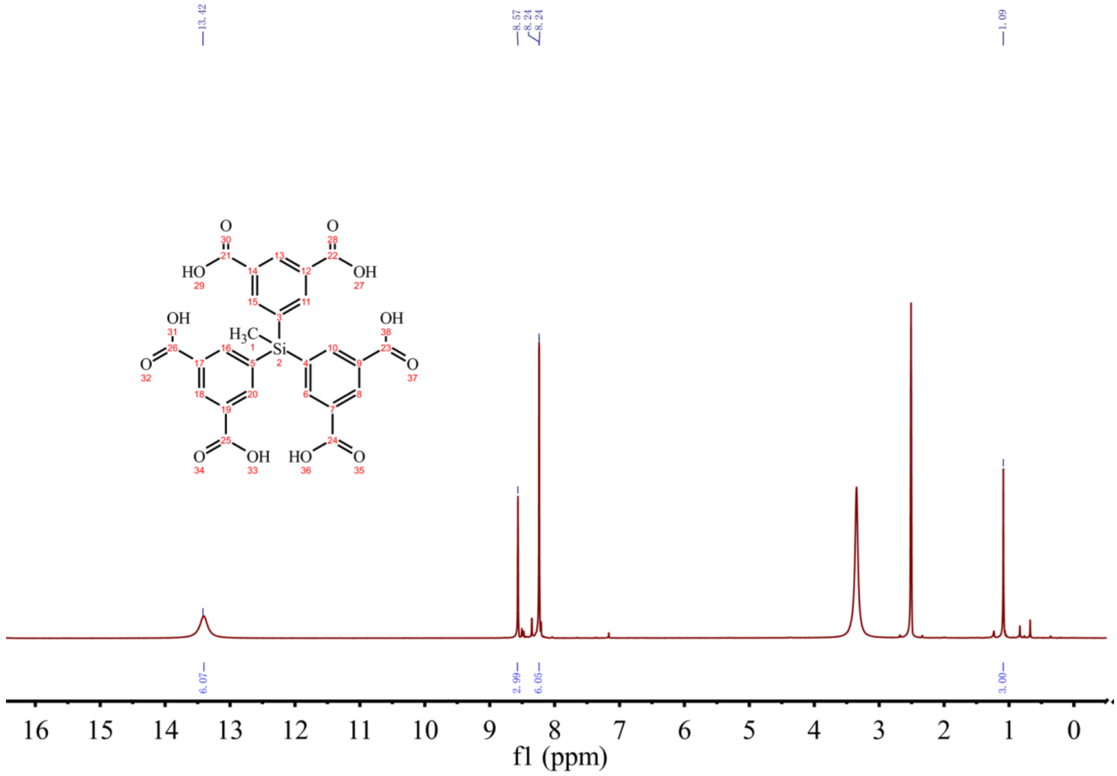

Figure S2 The ^{1}HNMR spectrum of 5,5',5''-(methylsilanetriyl)triisophthalic acid.

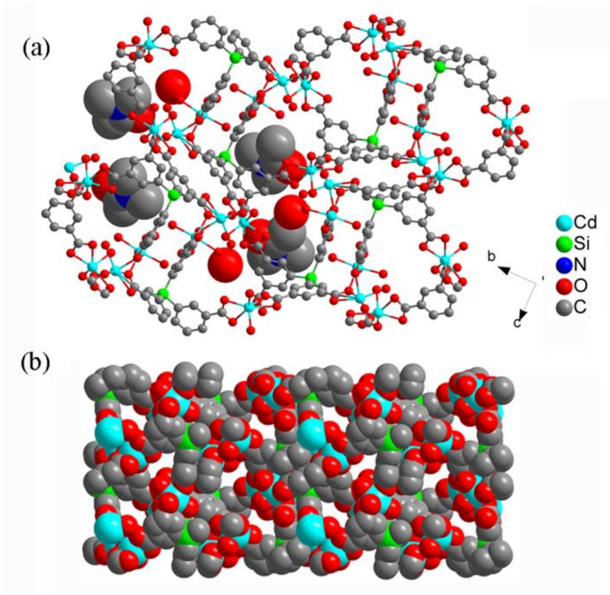

Figure S3 (a) View of the 3D framework in ‘ball and stick’ model, with guest molecules of DMF and H_2O residing in the channels. (b) The space-filling model of the framework viewing along the *a*-axis, wherein the guest molecules have been omitted for clarity.

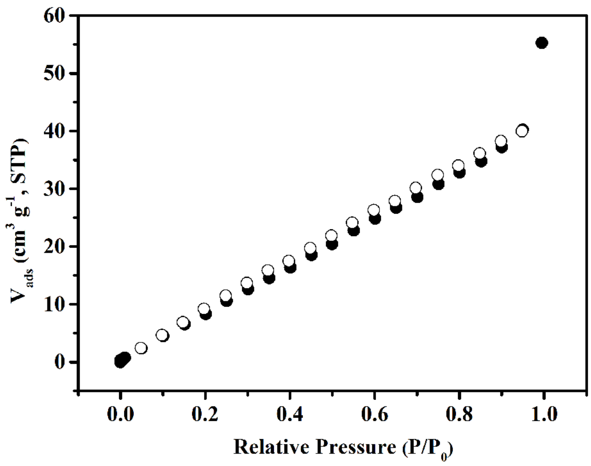

Figure S4 The N_2 sorption isotherm at 77K.

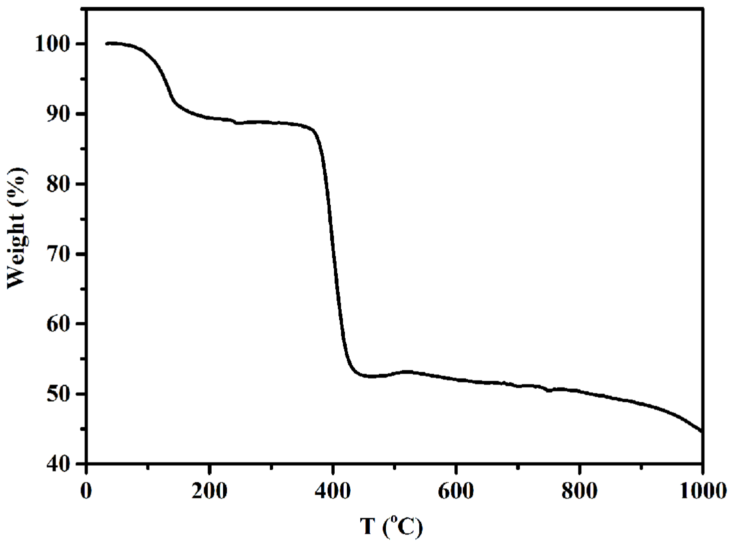

Figure S5 TG curve of compound **1**.

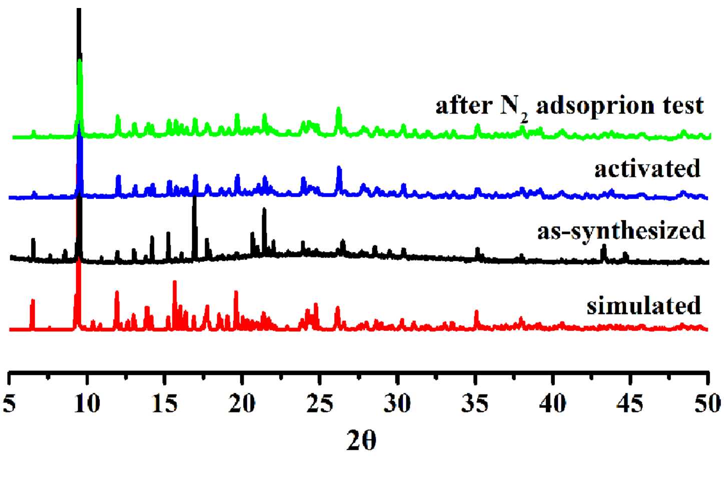

Figure S6 Powder X-ray diffraction patterns of simulated from the X-ray single structure of **1**, as-synthesized **1**, activated **1a** and sample after N_2 adsorption test.

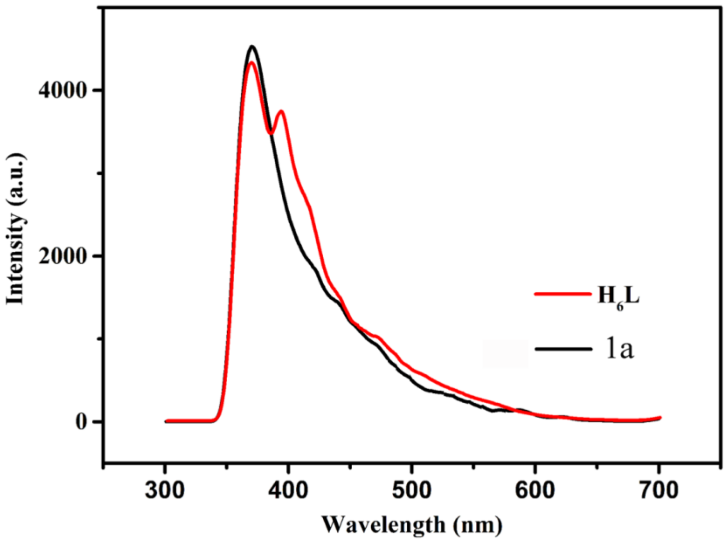

Figure S7 Solid state emission (λ_{ex} = 280 nm) spectra of **1a** and H_6L.

The luminescent spectra of compound **1** in the solid state showed emission bands at 370 nm. Compared with the free ligand of H_6L, compound **1** exhibits a little red-shift emission which could be assigned to the emissions of ligand-to-metal charge transfer (LMCT) and /or metal-to-ligand charge transfer (MLCT). [1]

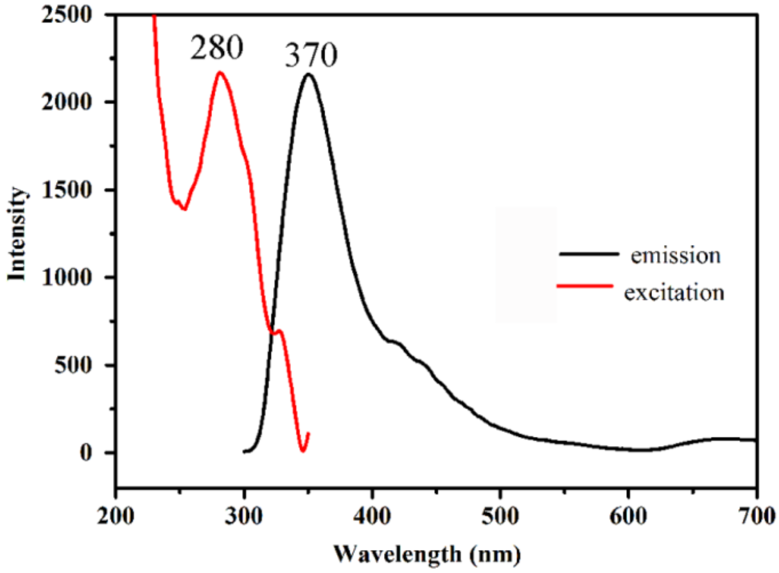

Figure S8 Solid state excitation (λ_{em} = 280 nm) and emission (λ_{ex} = 370 nm) spectra of **1**.

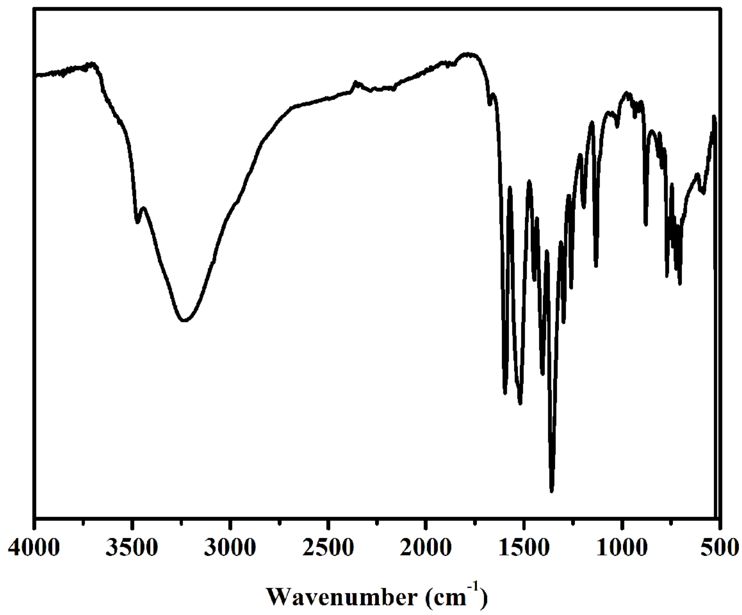

Figure S9 Infrared spectra of compound **1**.

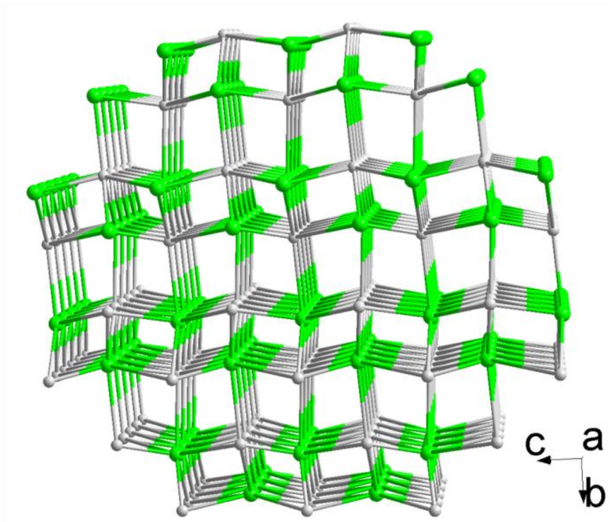

Figure S10 The simplified 6-connected topological net analyzed using TOPOS software.

1. F.-Y. Yi, Y. Wang, J.-P. Li, D. Wu, Y.-Q. Lan, Z.-M. Sun, *Mater. Horiz.* 2015, **2**, 245-251.