

Electronic Supplementary Information (ESI)

**Fluorescent Metal-organic Framework Based On Pyrene
Chromophore For Sensing of Nitrobenzene**

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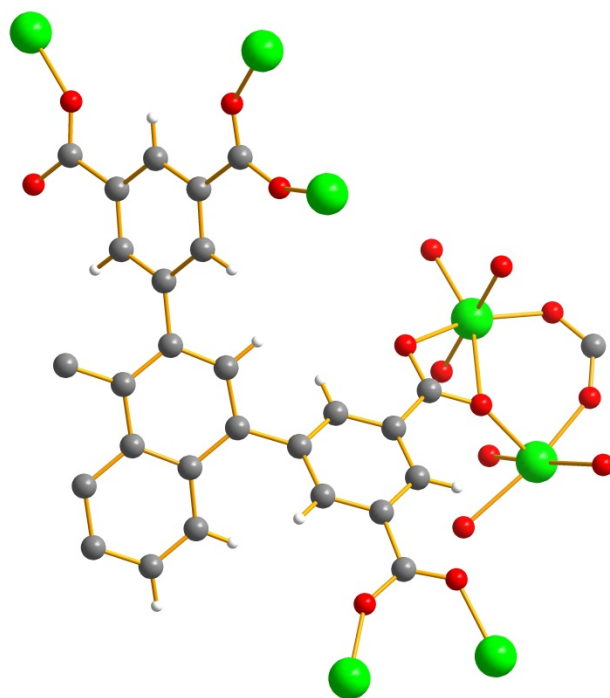


Fig S1. The asymmetric unit of **1**.

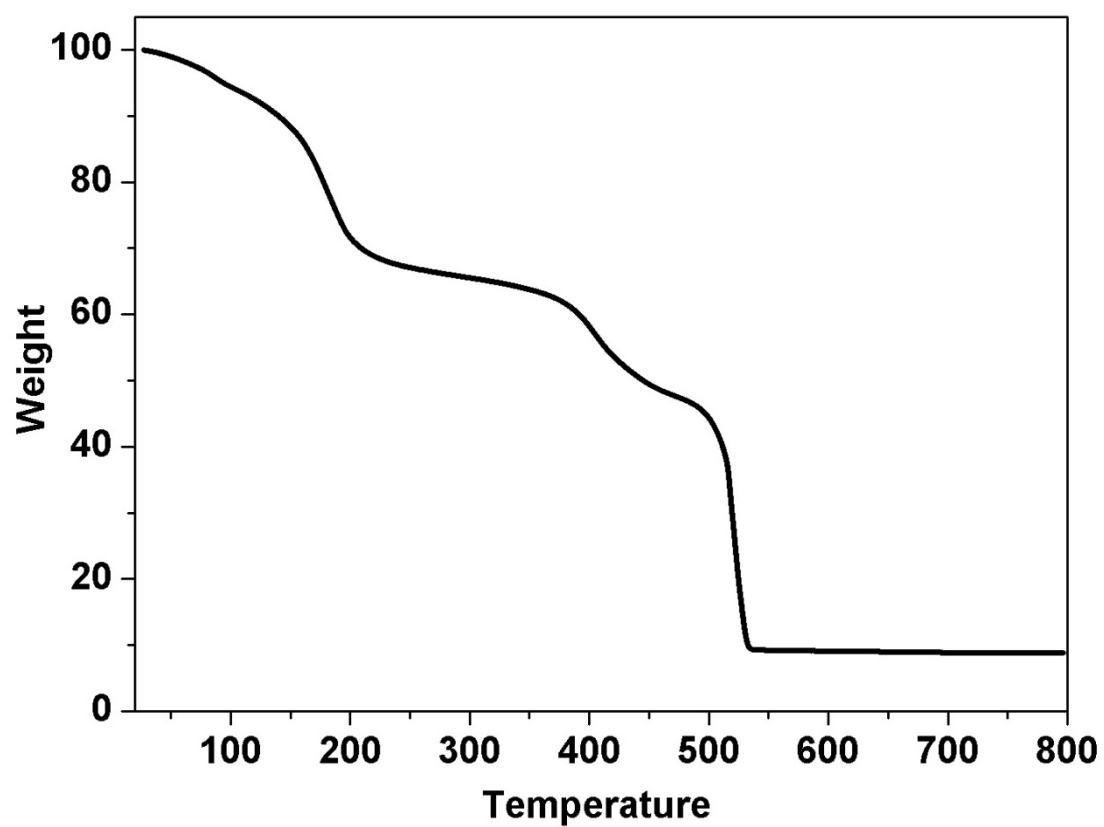


Fig S2. TGA analysis of **1**.

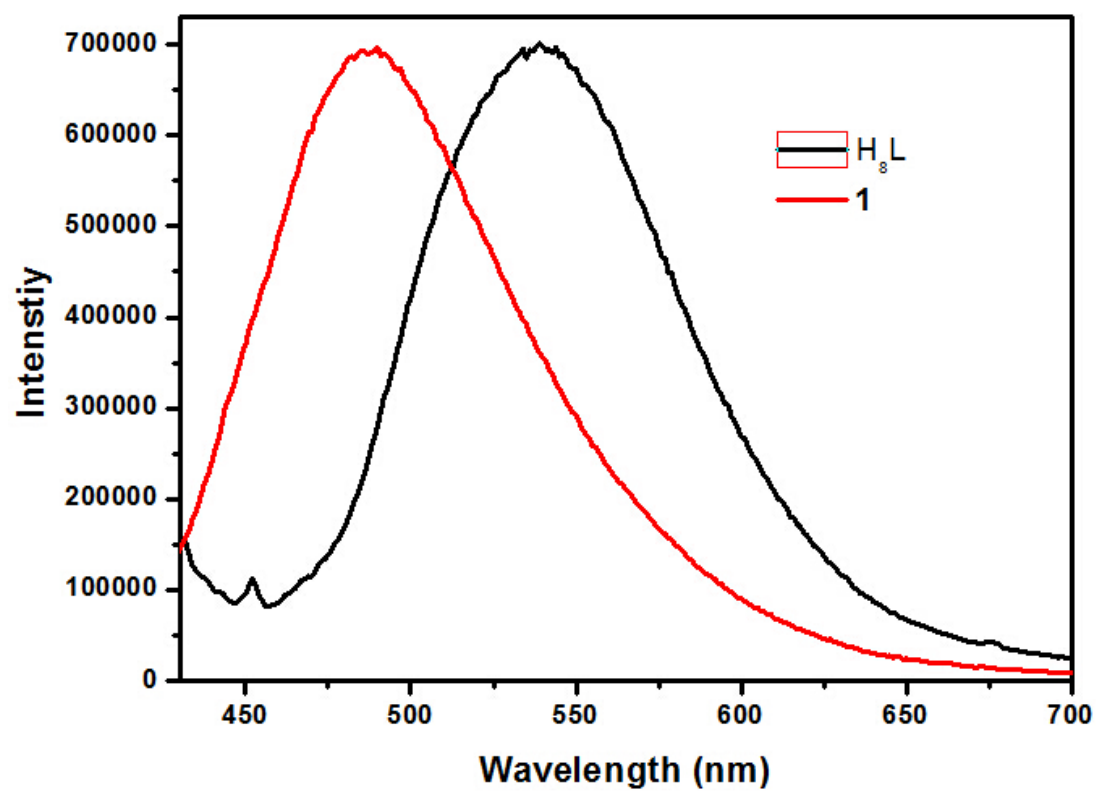


Fig S3. Emission spectrum of H_8L and **1**.

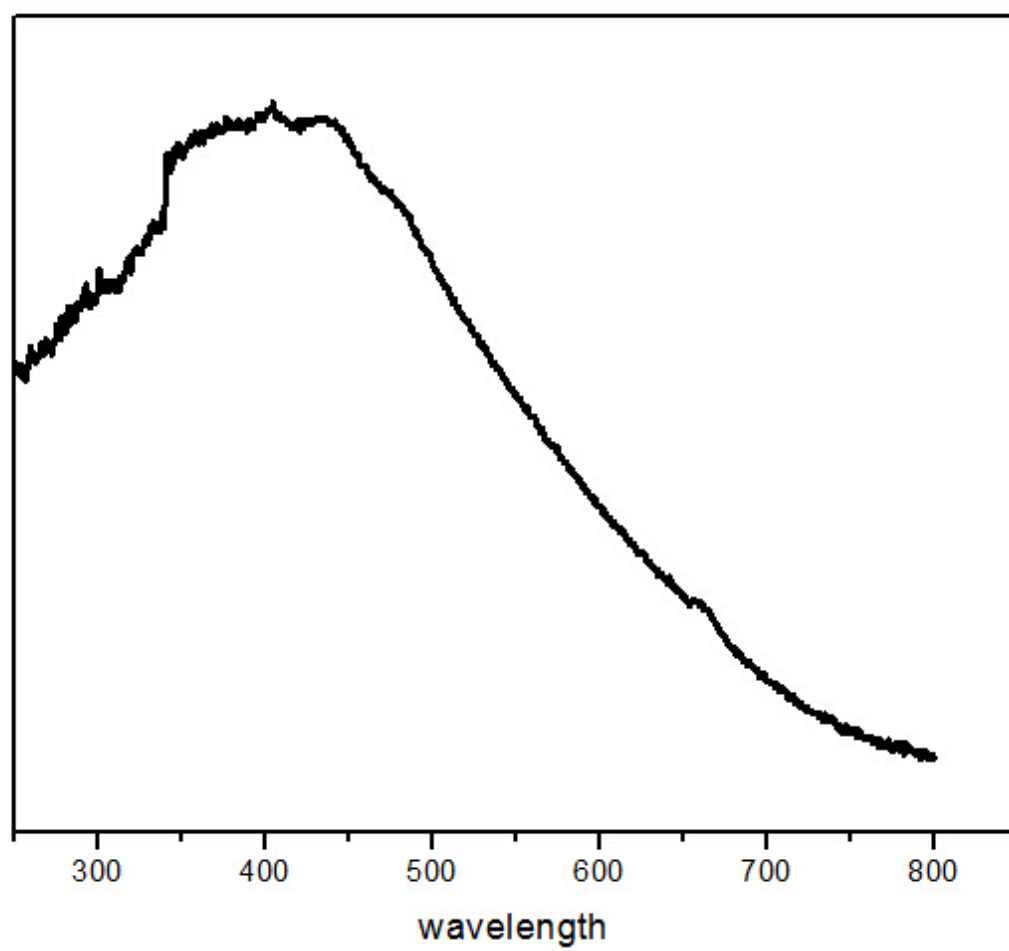


Fig S4. UV-Vis spectrum of **1**.

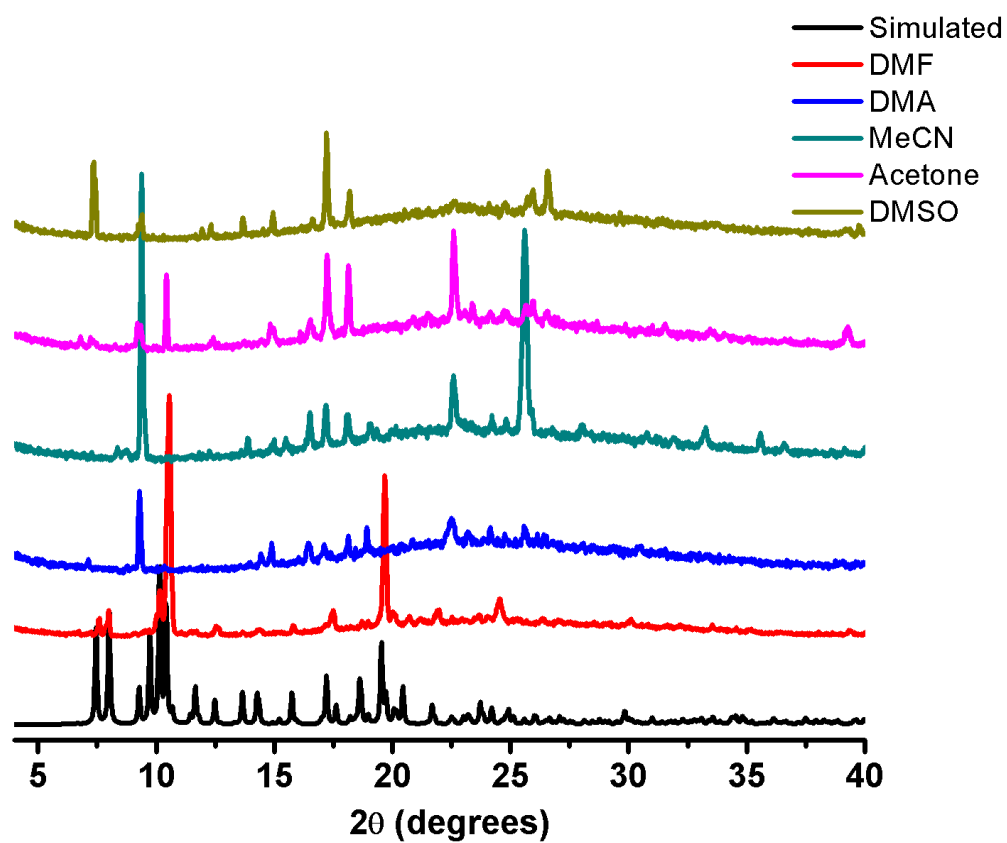


Figure S5. The PXRD of **1** in different common solvents.

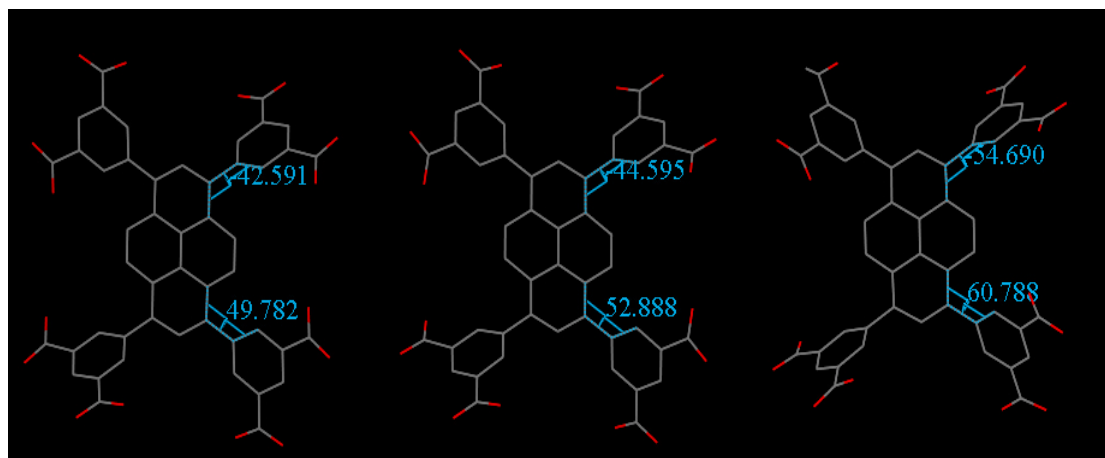


Figure S6. The different conformation of H_8L in **1** (left), JUC-118 (middle) and JUC-118-1 (right).

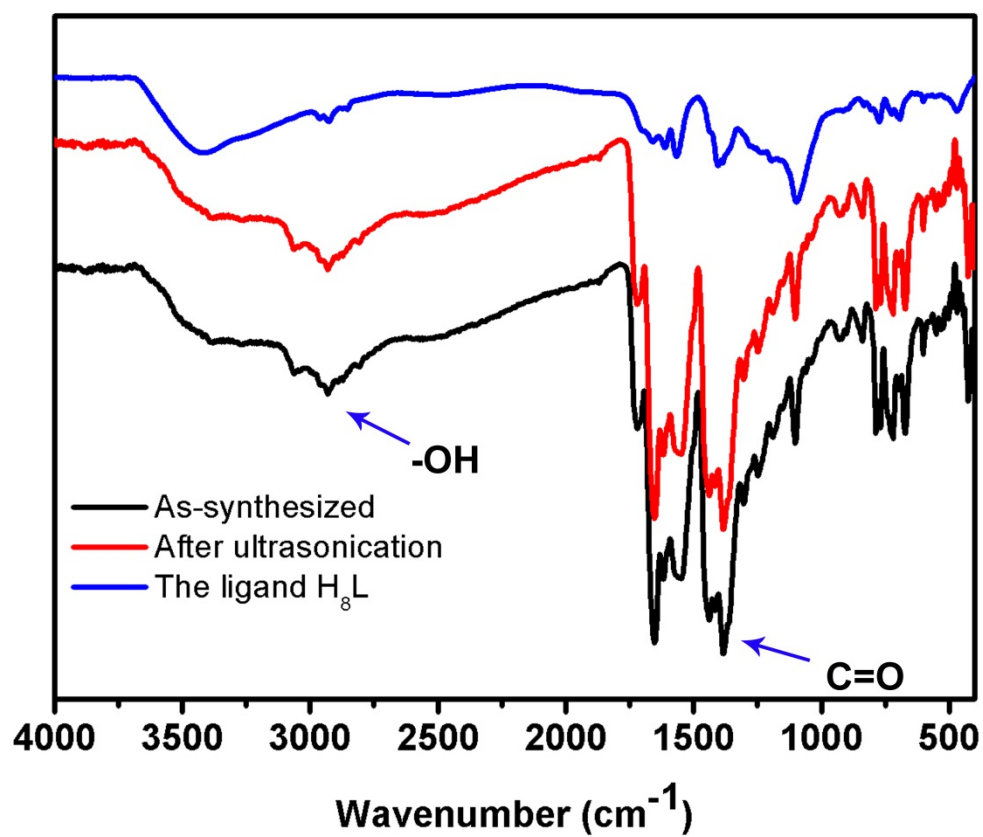


Figure S7. The IR spectrum of the ligand and **1** before and after ultrasonication treatment.

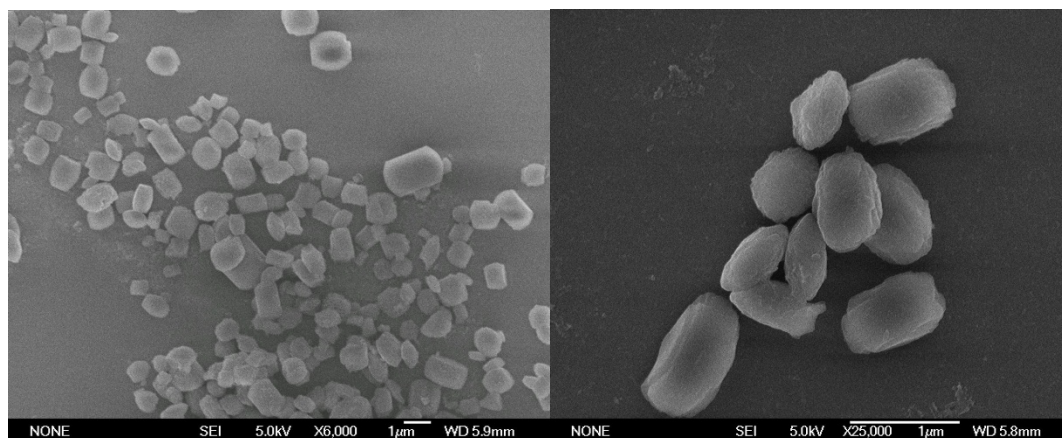


Figure S8. The SEM of **1** before (left) and after (right) ultrasonication treatment.

Table S1. Crystal data and structure refinement for 1.

Identification code	x	
Empirical formula	C _{30.75} H ₃₀ Mg ₂ N _{2.25} O _{12.75}	
Formula weight	683.69	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)/c	
Unit cell dimensions	a = 11.064(4) Å	α = 90 deg.
	b = 15.957(5) Å	β = 92.265(9) deg.
	c = 23.362(7) Å	γ = 90 deg.
Volume	4121(2) Å ³	
Z, Calculated density	4, 1.102 Mg/m ³	
Absorption coefficient	0.113 mm ⁻¹	
F(000)	1425	
Crystal size	0.15 x 0.15 x 0.1 mm	
Theta range for data collection	1.74 to 25.03 deg.	
Limiting indices	-12 ≤ h ≤ 13, -15 ≤ k ≤ 18, -27 ≤ l ≤ 27	
Reflections collected / unique	25991 / 7253 [R(int) = 0.0851]	
Completeness to theta = 25.03	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9888 and 0.9833	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7253 / 846 / 615	
Goodness-of-fit on F ²	0.997	

Final R indices [$I > 2\sigma(I)$]	R1 = 0.0991, wR2 = 0.2039
R indices (all data)	R1 = 0.1754, wR2 = 0.2371
Largest diff. peak and hole	0.454 and -0.292 e.Å ⁻³

Table S2. Bond lengths [Å] and angles [deg] for **1**.

Mg(1)-O(10)	1.885(11)
Mg(1)-O(8)#1	1.959(6)
Mg(1)-O(4)#2	1.966(6)
Mg(1)-O(12C)	1.995(11)
Mg(1)-O(1)	2.068(6)
Mg(1)-O(11)	2.118(9)
Mg(1)-O(11B)	2.184(14)
Mg(1)-O(12)	2.242(14)
Mg(1)-O(12B)	2.262(12)
Mg(1)-O(10B)	2.310(12)
Mg(1)-Mg(2)	3.600(3)
Mg(2)-O(3)#2	1.970(5)
Mg(2)-O(6)#3	1.970(4)
Mg(2)-O(7)#1	2.005(5)
Mg(2)-O(2)	2.066(5)
Mg(2)-O(9)	2.130(6)
Mg(2)-O(1)	2.460(6)
Mg(2)-C(1)	2.584(8)
O(1)-C(1)	1.252(7)
O(2)-C(1)	1.256(8)
O(3)-C(8)	1.220(8)
O(3)-Mg(2)#4	1.970(5)
O(4)-C(8)	1.267(8)
O(4)-Mg(1)#4	1.966(6)
O(5)-C(23)	1.252(7)
O(6)-C(23)	1.226(7)
O(6)-Mg(2)#3	1.970(4)
O(7)-C(24)	1.245(7)
O(7)-Mg(2)#5	2.005(5)
O(8)-C(24)	1.249(8)
O(8)-Mg(1)#5	1.959(6)
C(1)-C(2)	1.503(9)
C(2)-C(7)	1.374(7)
C(2)-C(3)	1.399(8)

C(3)-C(4)	1.387(8)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.398(7)
C(4)-C(8)	1.507(8)
C(5)-C(6)	1.392(7)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.385(7)
C(6)-C(9)	1.484(7)
C(7)-H(7A)	0.9300
C(9)-C(14)	1.398(7)
C(9)-C(10)	1.409(7)
C(10)-C(11)	1.433(7)
C(10)-C(15)	1.432(7)
C(11)-C(11)#6	1.426(9)
C(11)-C(12)	1.426(7)
C(12)-C(13)	1.401(7)
C(12)-C(16)#6	1.443(7)
C(13)-C(14)	1.378(7)
C(13)-C(17)	1.475(7)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.339(7)
C(15)-H(15A)	0.9300
C(16)-C(12)#6	1.443(7)
C(16)-H(16A)	0.9300
C(17)-C(22)	1.384(8)
C(17)-C(18)	1.395(7)
C(18)-C(19)	1.386(7)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.383(8)
C(19)-C(23)	1.510(8)
C(20)-C(21)	1.386(8)
C(20)-H(20A)	0.9300
C(21)-C(22)	1.384(7)
C(21)-C(24)	1.498(9)
C(22)-H(22A)	0.9300
O(11)-C(25)	1.172(15)
N(1)-C(25)	1.206(13)
N(1)-C(26)	1.401(13)
N(1)-C(27)	1.431(13)
C(25)-H(25A)	0.9300
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600

C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
O(11B)-C(25B)	1.165(17)
N(1B)-C(25B)	1.198(14)
N(1B)-C(26B)	1.410(14)
N(1B)-C(27B)	1.418(14)
C(25B)-H(25B)	0.9300
C(26B)-H(26D)	0.9600
C(26B)-H(26E)	0.9600
C(26B)-H(26F)	0.9600
C(27B)-H(27D)	0.9600
C(27B)-H(27E)	0.9600
C(27B)-H(27F)	0.9600
O(12)-C(28)	1.206(17)
N(2)-C(28)	1.188(16)
N(2)-C(30)	1.406(14)
N(2)-C(29)	1.420(15)
C(28)-H(28A)	0.9300
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
O(12B)-C(28B)	1.197(16)
N(2B)-C(28B)	1.192(15)
N(2B)-C(30B)	1.413(14)
N(2B)-C(29B)	1.421(14)
C(28B)-H(28B)	0.9300
C(29B)-H(29D)	0.9600
C(29B)-H(29E)	0.9600
C(29B)-H(29F)	0.9600
C(30B)-H(30D)	0.9600
C(30B)-H(30E)	0.9600
C(30B)-H(30F)	0.9600
N(3)-C(31)	1.201(17)
N(3)-C(32)	1.407(15)
N(3)-C(33)	1.409(15)
O(13)-C(31)	1.192(19)
C(31)-H(31A)	0.9300
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600

C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
O(14)-C(34)	1.196(13)
N(4)-C(34)	1.220(13)
N(4)-C(35)	1.394(12)
N(4)-C(36)	1.416(13)
C(34)-H(34A)	0.9300
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600

O(10)-Mg(1)-O(8)#1	160.4(4)
O(10)-Mg(1)-O(4)#2	105.9(4)
O(8)#1-Mg(1)-O(4)#2	93.4(3)
O(10)-Mg(1)-O(12C)	55.9(5)
O(8)#1-Mg(1)-O(12C)	104.5(5)
O(4)#2-Mg(1)-O(12C)	156.9(4)
O(10)-Mg(1)-O(1)	91.8(4)
O(8)#1-Mg(1)-O(1)	91.0(3)
O(4)#2-Mg(1)-O(1)	92.4(2)
O(12C)-Mg(1)-O(1)	101.5(5)
O(10)-Mg(1)-O(11)	88.7(5)
O(8)#1-Mg(1)-O(11)	84.9(4)
O(4)#2-Mg(1)-O(11)	98.3(4)
O(12C)-Mg(1)-O(11)	69.5(6)
O(1)-Mg(1)-O(11)	168.7(4)
O(10)-Mg(1)-O(11B)	87.4(8)
O(8)#1-Mg(1)-O(11B)	95.6(7)
O(4)#2-Mg(1)-O(11B)	71.0(6)
O(12C)-Mg(1)-O(11B)	92.6(7)
O(1)-Mg(1)-O(11B)	162.4(6)
O(11)-Mg(1)-O(11B)	28.9(6)
O(10)-Mg(1)-O(12)	85.9(14)
O(8)#1-Mg(1)-O(12)	75.0(14)
O(4)#2-Mg(1)-O(12)	167.9(15)
O(12C)-Mg(1)-O(12)	34.6(16)
O(1)-Mg(1)-O(12)	84.3(15)
O(11)-Mg(1)-O(12)	84.5(15)
O(11B)-Mg(1)-O(12)	113.1(16)
O(10)-Mg(1)-O(12B)	93.1(9)
O(8)#1-Mg(1)-O(12B)	67.5(8)

O(4)#2-Mg(1)-O(12B)	160.9(8)
O(12C)-Mg(1)-O(12B)	39.6(10)
O(1)-Mg(1)-O(12B)	88.2(10)
O(11)-Mg(1)-O(12B)	80.5(10)
O(11B)-Mg(1)-O(12B)	109.4(12)
O(12)-Mg(1)-O(12B)	8.3(17)
O(10)-Mg(1)-O(10B)	25.8(4)
O(8)#1-Mg(1)-O(10B)	172.5(5)
O(4)#2-Mg(1)-O(10B)	80.1(4)
O(12C)-Mg(1)-O(10B)	80.8(5)
O(1)-Mg(1)-O(10B)	93.0(5)
O(11)-Mg(1)-O(10B)	92.3(5)
O(11B)-Mg(1)-O(10B)	78.7(8)
O(12)-Mg(1)-O(10B)	111.6(14)
O(12B)-Mg(1)-O(10B)	118.9(9)
O(10)-Mg(1)-Mg(2)	125.8(4)
O(8)#1-Mg(1)-Mg(2)	66.34(16)
O(4)#2-Mg(1)-Mg(2)	62.91(18)
O(12C)-Mg(1)-Mg(2)	137.9(4)
O(1)-Mg(1)-Mg(2)	41.32(16)
O(11)-Mg(1)-Mg(2)	143.1(4)
O(11B)-Mg(1)-Mg(2)	128.3(6)
O(12)-Mg(1)-Mg(2)	108.2(17)
O(12B)-Mg(1)-Mg(2)	107.0(10)
O(10B)-Mg(1)-Mg(2)	113.3(4)
O(3)#2-Mg(2)-O(6)#3	103.3(2)
O(3)#2-Mg(2)-O(7)#1	95.7(2)
O(6)#3-Mg(2)-O(7)#1	91.7(2)
O(3)#2-Mg(2)-O(2)	157.8(2)
O(6)#3-Mg(2)-O(2)	97.6(2)
O(7)#1-Mg(2)-O(2)	91.1(2)
O(3)#2-Mg(2)-O(9)	87.0(2)
O(6)#3-Mg(2)-O(9)	90.3(2)
O(7)#1-Mg(2)-O(9)	176.1(2)
O(2)-Mg(2)-O(9)	85.4(2)
O(3)#2-Mg(2)-O(1)	101.6(2)
O(6)#3-Mg(2)-O(1)	154.9(2)
O(7)#1-Mg(2)-O(1)	89.4(2)
O(2)-Mg(2)-O(1)	57.24(18)
O(9)-Mg(2)-O(1)	87.3(2)
O(3)#2-Mg(2)-C(1)	130.1(2)
O(6)#3-Mg(2)-C(1)	126.3(2)
O(7)#1-Mg(2)-C(1)	89.1(2)
O(2)-Mg(2)-C(1)	28.68(19)

O(9)-Mg(2)-C(1)	87.0(2)
O(1)-Mg(2)-C(1)	28.61(17)
O(3)#2-Mg(2)-Mg(1)	74.72(18)
O(6)#3-Mg(2)-Mg(1)	163.60(18)
O(7)#1-Mg(2)-Mg(1)	72.49(14)
O(2)-Mg(2)-Mg(1)	87.33(16)
O(9)-Mg(2)-Mg(1)	105.70(19)
O(1)-Mg(2)-Mg(1)	33.70(13)
C(1)-Mg(2)-Mg(1)	59.57(17)
C(1)-O(1)-Mg(1)	147.5(5)
C(1)-O(1)-Mg(2)	81.2(5)
Mg(1)-O(1)-Mg(2)	105.0(2)
C(1)-O(2)-Mg(2)	99.2(4)
C(8)-O(3)-Mg(2)#4	127.2(5)
C(8)-O(4)-Mg(1)#4	145.9(5)
C(23)-O(6)-Mg(2)#3	139.1(5)
C(24)-O(7)-Mg(2)#5	130.7(5)
C(24)-O(8)-Mg(1)#5	141.2(6)
O(1)-C(1)-O(2)	122.2(7)
O(1)-C(1)-C(2)	119.7(7)
O(2)-C(1)-C(2)	118.2(6)
O(1)-C(1)-Mg(2)	70.2(4)
O(2)-C(1)-Mg(2)	52.1(4)
C(2)-C(1)-Mg(2)	169.6(5)
C(7)-C(2)-C(3)	120.0(6)
C(7)-C(2)-C(1)	117.9(6)
C(3)-C(2)-C(1)	122.1(6)
C(4)-C(3)-C(2)	119.2(5)
C(4)-C(3)-H(3A)	120.4
C(2)-C(3)-H(3A)	120.4
C(3)-C(4)-C(5)	120.0(5)
C(3)-C(4)-C(8)	120.5(6)
C(5)-C(4)-C(8)	119.4(6)
C(6)-C(5)-C(4)	120.7(5)
C(6)-C(5)-H(5A)	119.6
C(4)-C(5)-H(5A)	119.6
C(7)-C(6)-C(5)	118.3(5)
C(7)-C(6)-C(9)	119.8(5)
C(5)-C(6)-C(9)	121.9(5)
C(2)-C(7)-C(6)	121.7(5)
C(2)-C(7)-H(7A)	119.1
C(6)-C(7)-H(7A)	119.1
O(3)-C(8)-O(4)	126.1(7)
O(3)-C(8)-C(4)	118.0(7)

O(4)-C(8)-C(4)	115.8(6)
C(14)-C(9)-C(10)	118.8(5)
C(14)-C(9)-C(6)	118.0(5)
C(10)-C(9)-C(6)	123.2(5)
C(9)-C(10)-C(11)	118.9(5)
C(9)-C(10)-C(15)	123.0(5)
C(11)-C(10)-C(15)	118.1(5)
C(11)#6-C(11)-C(12)	120.4(6)
C(11)#6-C(11)-C(10)	119.6(5)
C(12)-C(11)-C(10)	120.0(4)
C(13)-C(12)-C(11)	119.6(5)
C(13)-C(12)-C(16)#6	122.6(5)
C(11)-C(12)-C(16)#6	117.8(4)
C(14)-C(13)-C(12)	119.1(5)
C(14)-C(13)-C(17)	118.0(5)
C(12)-C(13)-C(17)	122.8(5)
C(13)-C(14)-C(9)	123.2(5)
C(13)-C(14)-H(14A)	118.4
C(9)-C(14)-H(14A)	118.4
C(16)-C(15)-C(10)	122.1(5)
C(16)-C(15)-H(15A)	119.0
C(10)-C(15)-H(15A)	119.0
C(15)-C(16)-C(12)#6	121.6(5)
C(15)-C(16)-H(16A)	119.2
C(12)#6-C(16)-H(16A)	119.2
C(22)-C(17)-C(18)	118.0(5)
C(22)-C(17)-C(13)	119.2(5)
C(18)-C(17)-C(13)	122.8(5)
C(19)-C(18)-C(17)	120.9(6)
C(19)-C(18)-H(18A)	119.5
C(17)-C(18)-H(18A)	119.5
C(20)-C(19)-C(18)	120.0(5)
C(20)-C(19)-C(23)	119.3(5)
C(18)-C(19)-C(23)	120.7(6)
C(19)-C(20)-C(21)	119.8(5)
C(19)-C(20)-H(20A)	120.1
C(21)-C(20)-H(20A)	120.1
C(22)-C(21)-C(20)	119.7(6)
C(22)-C(21)-C(24)	119.5(6)
C(20)-C(21)-C(24)	120.8(6)
C(21)-C(22)-C(17)	121.6(6)
C(21)-C(22)-H(22A)	119.2
C(17)-C(22)-H(22A)	119.2
O(6)-C(23)-O(5)	125.3(6)

O(6)-C(23)-C(19)	117.1(6)
O(5)-C(23)-C(19)	117.6(5)
O(7)-C(24)-O(8)	125.6(7)
O(7)-C(24)-C(21)	118.6(6)
O(8)-C(24)-C(21)	115.8(6)
C(25)-O(11)-Mg(1)	131.4(15)
C(25)-N(1)-C(26)	128.8(13)
C(25)-N(1)-C(27)	121.5(13)
C(26)-N(1)-C(27)	109.6(12)
O(11)-C(25)-N(1)	140.1(18)
O(11)-C(25)-H(25A)	110.0
N(1)-C(25)-H(25A)	110.0
N(1)-C(26)-H(26A)	109.5
N(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(1)-C(27)-H(27A)	109.5
N(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25B)-O(11B)-Mg(1)	117.2(19)
C(25B)-N(1B)-C(26B)	128.1(14)
C(25B)-N(1B)-C(27B)	122.5(14)
C(26B)-N(1B)-C(27B)	109.4(14)
O(11B)-C(25B)-N(1B)	146(3)
O(11B)-C(25B)-H(25B)	106.9
N(1B)-C(25B)-H(25B)	106.9
N(1B)-C(26B)-H(26D)	109.5
N(1B)-C(26B)-H(26E)	109.5
H(26D)-C(26B)-H(26E)	109.5
N(1B)-C(26B)-H(26F)	109.5
H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5
N(1B)-C(27B)-H(27D)	109.5
N(1B)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
N(1B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(28)-O(12)-Mg(1)	165(4)

C(28)-N(2)-C(30)	126.4(15)
C(28)-N(2)-C(29)	125.2(14)
C(30)-N(2)-C(29)	108.4(14)
N(2)-C(28)-O(12)	137(3)
N(2)-C(28)-H(28A)	111.7
O(12)-C(28)-H(28A)	111.7
N(2)-C(29)-H(29A)	109.5
N(2)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
N(2)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(2)-C(30)-H(30A)	109.5
N(2)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
N(2)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(28B)-O(12B)-Mg(1)	151(3)
C(28B)-N(2B)-C(30B)	126.4(13)
C(28B)-N(2B)-C(29B)	124.4(14)
C(30B)-N(2B)-C(29B)	109.2(13)
N(2B)-C(28B)-O(12B)	138(2)
N(2B)-C(28B)-H(28B)	110.8
O(12B)-C(28B)-H(28B)	110.8
N(2B)-C(29B)-H(29D)	109.5
N(2B)-C(29B)-H(29E)	109.5
H(29D)-C(29B)-H(29E)	109.5
N(2B)-C(29B)-H(29F)	109.5
H(29D)-C(29B)-H(29F)	109.5
H(29E)-C(29B)-H(29F)	109.5
N(2B)-C(30B)-H(30D)	109.5
N(2B)-C(30B)-H(30E)	109.5
H(30D)-C(30B)-H(30E)	109.5
N(2B)-C(30B)-H(30F)	109.5
H(30D)-C(30B)-H(30F)	109.5
H(30E)-C(30B)-H(30F)	109.5
C(31)-N(3)-C(32)	125.2(15)
C(31)-N(3)-C(33)	123.7(15)
C(32)-N(3)-C(33)	111.0(16)
O(13)-C(31)-N(3)	134(3)
O(13)-C(31)-H(31A)	112.9
N(3)-C(31)-H(31A)	112.9
N(3)-C(32)-H(32A)	109.5

N(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(3)-C(33)-H(33A)	109.5
N(3)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
N(3)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(34)-N(4)-C(35)	126.9(11)
C(34)-N(4)-C(36)	120.9(11)
C(35)-N(4)-C(36)	112.1(12)
O(14)-C(34)-N(4)	130.9(14)
O(14)-C(34)-H(34A)	114.5
N(4)-C(34)-H(34A)	114.5
N(4)-C(35)-H(35A)	109.5
N(4)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
N(4)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
N(4)-C(36)-H(36A)	109.5
N(4)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
N(4)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5