Table S1. Selected Bond Lengths (Å) and Bond Angles (°) of **1**.

Bond	Dist.	Bond	Dist.
Ho(1)-O(7)	2.361(4)	Ho(1)-O(1)	2.275(4)
Ho(1)-O(3)$^{\#1}$	2.372(4)	Ho(1)-O(10)	2.348(4)
Ho(1)-O(8)	2.594(4)	Ho(1)-O(5)$^{\#2}$	2.307(4)
Ho(1)-O(9)	2.316(4)	Ho(1)-O(2)$^{\#1}$	2.336(4)
Ho(2)-O(4)	2.426(4)	Ho(2)-O(16)	2.355(4)
Ho(2)-O(21)	2.238(4)	Ho(2)-O(15)$^{\#4}$	2.363(4)
Ho(2)-O(17)	2.500(4)	Ho(2)-O(6)	2.283(4)
Ho(2)-O(20)	2.379(5)	Ho(2)-O(19)	2.364(5)
Angle	**(°)**	**Angle**	**(°)**
O(7)-Ho(1)-O(3)$^{\#1}$	140.86(14)	O(7)-Ho(1)-O(8)	138.59(14)
O(3)#1-Ho(1)-O(8)	74.73(14)	O(1)-Ho(1)-O(7)	76.21(15)
O(1)-Ho(1)-O(3)$^{\#1}$	142.39(14)	O(1)-Ho(1)-O(8)	75.56(14)
O(1)-Ho(1)-O(10)	146.96(15)	O(1)-Ho(1)-O(5)$^{\#2}$	78.99(15)
O(1)-Ho(1)-O(9)	98.93(17)	O(1)-Ho(1)-O(2)$^{\#1}$	79.84(14)
O(10)-Ho(1)-O(7)	73.40(14)	O(10)-Ho(1)-O(3)$^{\#1}$	69.92(14)
O(10)-Ho(1)-O(8)	121.22(14)	O(5)$^{\#2}$-Ho(1)-O(7)	73.12(15)
O(5)$^{\#2}$-Ho(1)-O(3)$^{\#1}$	112.67(15)	O(5)$^{\#2}$-Ho(1)-O(8)	72.23(14)
O(5)$^{\#2}$-Ho(1)-O(10)	80.06(14)	O(5)$^{\#2}$-Ho(1)-O(2)$^{\#1}$	142.56(14)
O(5)$^{\#2}$-Ho(1)-O(9)	143.50(15)	O(9)-Ho(1)-O(3)$^{\#1}$	91.32(16)
O(9)-Ho(1)-O(7)	71.06(15)	O(9)-Ho(1)-O(10)	83.28(16)
O(9)-Ho(1)-O(8)	143.15(14)	O(2)$^{\#1}$-Ho(1)-O(7)	130.17(14)
O(9)-Ho(1)-O(2)$^{\#1}$	70.40(15)	O(2)$^{\#1}$-Ho(1)-O(8)	72.77(13)
O(2)$^{\#1}$-Ho(1)-O(3)$^{\#1}$	69.71(13)	O(4)-Ho(2)-O(17)	151.07(15)
O(2)$^{\#1}$-Ho(1)-O(10)	130.58(14)	O(16)-Ho(2)-O(4)	143.74(14)
O(4)-Ho(2)-C(17)	159.79(16)	O(16)-Ho(2)-O(17)	53.37(14)
O(16)-Ho(2)-O(15)$^{\#4}$	73.16(15)	O(16)-Ho(2)-O(19)	87.51(17)
O(16)-Ho(2)-O(20)	93.15(19)	O(21)-Ho(2)-O(4)	81.88(15)
O(16)-Ho(2)-C(17)	27.10(16)	O(21)-Ho(2)-O(15)$^{\#4}$	80.82(17)
O(21)-Ho(2)-O(16)	92.06(16)	O(21)-Ho(2)-O(6)	114.98(16)
O(21)-Ho(2)-O(17)	125.92(16)	O(21)-Ho(2)-O(19)	157.66(18)
O(21)-Ho(2)-O(20)	72.24(18)	O(15)$^{\#4}$-Ho(2)-O(4)	70.58(14)
O(21)-Ho(2)-C(17)	111.06(17)	O(15)$^{\#4}$-Ho(2)-O(20)	149.37(17)
O(15)$^{\#4}$-Ho(2)-O(17)	117.36(15)	O(6)-Ho(2)-O(4)	70.41(14)
O(15)$^{\#4}$-Ho(2)-O(19)	77.67(18)	O(6)-Ho(2)-O(15)$^{\#4}$	134.78(15)
O(15)$^{\#4}$-Ho(2)-C(17)	95.51(16)	O(6)-Ho(2)-O(20)	71.89(18)
O(6)-Ho(2)-O(16)	141.71(15)	O(20)-Ho(2)-O(4)	118.30(18)
O(6)-Ho(2)-O(17)	88.36(14)	O(19)-Ho(2)-O(4)	85.30(16)
O(6)-Ho(2)O(19)	77.24(18)	O(19)-Ho(2)-O(20)	130.10(18)
O(20)-Ho(2)-O(17)	70.29(18)	O(19)-Ho(2)-O(17)	70.60(17)

Symmetry codes: #1: -x+1, -y+2, -z+2; #2: x-1, y, z; #4: –x, 1-y, 1-z.

Table S2. Hydrogen Bond Length (A) and Bond Angle (°) of **1.**

D-H...A	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6)···O(8)[a]	2.43	3.344(6)	166.8
C(19)-H(19)···(22)[a]	2.66	3.559(7)	164
C(13)-H(13A)···O(24)[d]	2.63	3.508(8)	158.3
O(24)-H(24A)···O(14)[b]	1.97(2)	2.804(7)	172.(7)
O(24)-H(24B)···O(6)[c]	2.55(7)	3.032(7)	117.(6)
O(24)-H(24B)···O(23)	2.29(4)	3.050(7)	150.(7)
O(13)-H(13)···O(16)[b]	2.55(4)	3.177(6)	126.(4)
O(24)-H(24B)···O(23)	2.29(4)	3.050(7)	150.(7)
O(13)-H(13)···O(15)	1.72(3)	2.570(6)	154.(4)
O(12)-H(12)···O(7)	2.44(4)	3.028(6)	126.(4)
O(12)-H(12)···O(10)	1.79(4)	2.570(6)	151.(5)
O(8)-H(8A)···O(11)[d]	2.00(4)	2.854(6)	153.(8)
O(8)-H(8B)···O(2)	1.98(5)	2.771(5)	144.(8)
O(9)-H(9A)···O(22)[e]	1.85(4)	2.695(6)	151.(7)
O(9)-H(9B)···O(13)[f]	2.65(7)	3.274(6)	125.(7)
O(9)-H(9B)···O(18)[g]	1.84(5)	2.698(6)	152.(9)
O(7)-H(7A)···O(13)[f]	1.85(2)	2.774(6)	178.(10)
O(7)-H(7B)···O(24)	1.77(3)	2.685(7)	168.(9)
O(19)-H(19A)···O(12)[f]	1.87(4)	2.767(7)	161.(9)
O(19)-H(19B)···O(24)[f]	2.15(6)	2.994(8)	151.(10)
O(20)-H(20A)···O(8)[h]	2.08(2)	2.999(7)	177.(10)
O(20)-H(20B)···O(23)[f]	2.45(6)	3.219(7)	141.(7)
O(18)-H(18)···O(13)[i]	2.57(8)	2.994(6)	115.(7)
O(18)-H(18)···O(16)[j]	1.87(9)	2.581(6)	149.(8)
O(4)-H(4)···O(14)[b]	1.73(6)	2.514(6)	161.(6)
O(23)-H(23)···O(22)	1.94(8)	2.594(7)	163.(9)
O(3)-H(3)···O(11)[k]	1.73(10)	2.564(5)	166.(10)

Symmetry codes: a: x+1, y, z; b: -x, 1-y, 1-z; c: x-1, y, z; d: -x, 2-y, 2-z; e: x, y+1, z; f: x+1, y, z; g: x-1, y+1, z; h: –x+1, -y+1, -z+2; i: x+2, y-1, z; j: –x+2, -y, -z+1; k -x+1, -y+2, -z+2.

Table S3. Short Ring-Interactions with Cg-Cg Distances < 4.0 Å, α < 20.000° and β < 60.0°. And the Analysis of C-H···Cg (π-Ring) Interactions (H···Cg < 3.0 Å. γ < 30.0°) for **1**.

Cg(I)	Cg(J)[ARU]	Cg-Cg	Transformed J-Plane				α	β	γ	CgI_Perp	CgJ_Perp	Slippage
			P	Q	R	S						
Cg(1)	Cg(4)[II]	3.742(3)	0.1524	0.8020	-0.5776	-4.7521	5.5(3)	29.9	26.6	3.345(2)	3.244(2)	1.865
Cg(1)	Cg(4) [III]	3.742(3)	-0.1524	-0.8020	0.5776	4.7521	5.5(3)	29.9	26.6	3.345(2)	3.244(2)	1.865
Cg2	Cg3[IV]	3.731(3)	0.1925	0.7390	-0.6456	2.4974	6.0(3)	23.3	29.2	3.258(2)	3.427(2)	1.475
Cg2	Cg3[V]	3.731(3)	0.1925	-0.7390	0.6456	-2.4974	6.0(3)	23.3	29.2	3.258(2)	3.427(2)	1.475
Cg3	Cg2[VI]	3.730(3)	0.2803	0.7553	-0.5924	-5.6914	6.0(3)	29.2	23.3	3.427(2)	3.257(2)	1.818
Cg3	Cg2[V]	3.730(3)	0.2803	-0.7553	0.5924	-1.1621	6.0(3)	29.2	23.3	3.427(2)	3.257(2)	1.818
Cg4	Cg1[II]	3.741(3)	0.1512	0.7427	-0.652	-2.657	5.5(3)	26.6	29.9	3.244(2)	3.345(2)	1.677
Cg4	Cg1[III]	3.742(3)	0.1512	-0.7427	0.6524	9.1459	5.5(3)	26.6	26.6	3.245(2)	3.345(2)	1.677
C(I)-H(I)	Cg(J)[ARU]	C···Cg	P	Q	R	S	H-Perp	γ	C-H···Cg	H···Cg	C-H,π	C(I)-H(I)
C(9)-O(11)	Cg1[III]	3.371(5)	0.1512	0.7427	0.6524	-4.1184	3.213	17.60	75.0(3)	3.278(6)	0.79	C(9)-O(11)
C(16)-O(14)	Cg2 [VII]	3.850(5)	-0.2803	-0.7553	0.5924	4.2534	-3.498	24.66	111.2(4)	4.464(6)	1.55	C(16)-O(14)