Electronic Supplementary Information

Mesostructured molecular solid material $|Co(en)_3|(Zr_2F_{11}H_2O)$ with enhanced photoelectronic effect

Yu Du[a,b], Jihong Yu[c], Yuan Chen[a], and Yanhui Yang[a]*

[a] School of Chemical & Biomedical Engineering, Nanyang Technological University, 637459 Singapore, Singapore

[b] College of Electronic Science & Engineering, Jilin University, Changchun 130012 P. R. China.

[c] State Key Laboratory of Inorganic Synthesis and Preparative Chemistry. College of Chemistry, Jilin University, Changchun 130012 P. R. China.

Table S1

Atom	X	Y	Z	U(eq)
Zr(1)	934(1)	1048(1)	4597(1)	20(1)
Zr(2)	2438(1)	3214(1)	3858(1)	19(1)
Co(1)	3111(1)	6917(1)	3322(1)	20(1)
F(1)	-1275(4)	315(2)	4901(2)	27(1)
F(2)	325(4)	360(2)	3374(2)	29(1)
F(3)	3238(4)	882(3)	4700(3)	41(1)
F(4)	-997(4)	1877(2)	4325(3)	32(1)
F(5)	1896(5)	2395(2)	5044(2)	30(1)
F(6)	1541(5)	1907(2)	3431(2)	31(1)
F(7)	226(4)	3627(3)	3551(3)	38(1)
F(8)	2974(5)	3957(2)	5038(3)	32(1)
F(9)	4753(4)	2793(2)	4080(3)	31(1)
F(10)	2670(5)	3034(2)	2418(2)	31(1)
F(11)	3158(6)	4403(3)	3368(3)	47(1)
O(1)	817(6)	1173(3)	6146(3)	30(1)
C(1)	2900(10)	8735(5)	2776(6)	45(2)
C(2)	3863(10)	8732(5)	3720(5)	41(2)
C(3)	391(8)	6099(5)	3935(5)	34(2)
C(4)	1684(8)	6032(5)	4773(5)	33(2)
C(5)	4422(8)	5874(4)	1936(5)	30(2)
C(6)	5738(8)	5952(4)	2761(5)	31(2)
N(1)	2910(6)	7839(3)	2328(4)	25(1)
N(2)	3450(6)	7921(4)	4232(4)	28(1)
N(3)	777(6)	6902(4)	3370(4)	29(1)
N(4)	3228(6)	6039(3)	4368(4)	26(1)
N(5)	2882(6)	5993(3)	2342(4)	24(1)
N(6)	5418(6)	6783(3)	3285(4)	25(1)

Table S2

Zr(1)-F(3)	1.945(4)	Co(1)-N(5)	1.949(5)
Zr(1)-F(2)	2.020(3)	Co(1)-N(1)	1.961(5)
Zr(1)-F(4)	2.044(4)	Co(1)-N(6)	1.962(5)
Zr(1)-F(1)#1	2.167(3)	Co(1)-N(4)	1.970(5)
Zr(1)-F(6)	2.200(4)	Co(1)-N(2)	1.973(5)
Zr(1)-O(1)	2.210(5)	Co(1)-N(3)	1.976(5)
Zr(1)-F(5)	2.234(3)	F(1)-Zr(1)#1	2.167(3)
Zr(1)-F(1)	2.247(4)	C(1)-C(2)	1.471(10)
Zr(1)-Zr(2)	3.6795(8)	C(1)-N(1)	1.484(9)
Zr(2)-F(7)	1.960(4)	C(2)-N(2)	1.477(9)
Zr(2)-F(8)	2.008(3)	C(3)-N(3)	1.501(8)
Zr(2)-F(11)	2.029(4)	C(3)-C(4)	1.507(9)
Zr(2)-F(9)	2.037(4)	C(4)-N(4)	1.486(8)
Zr(2)-F(10)	2.085(3)	C(5)-N(5)	1.493(8)
Zr(2)-F(6)	2.156(3)	C(5)-C(6)	1.509(9)
Zr(2)-F(5)	2.170(3)	C(6)-N(6)	1.489(8)
F(3)-Zr(1)-F(2)	98.19(17)	F(8)-Zr(2)-F(6)	140.28(14)
F(3)-Zr(1)-F(4)	148.81(16)	F(11)-Zr(2)-F(6)	144.08(15)
F(2)-Zr(1)-F(4)	92.22(15)	F(9)-Zr(2)-F(6)	93.28(15)
F(3)-Zr(1)-F(1)#1	76.40(15)	F(10)-Zr(2)-F(6)	71.46(14)
F(2)-Zr(1)-F(1)#1	78.99(14)	F(7)-Zr(2)-F(5)	93.54(15)
F(4)-Zr(1)-F(1)#1	134.64(14)	F(8)-Zr(2)-F(5)	73.68(14)
F(3)-Zr(1)-F(6)	78.86(16)	F(11)-Zr(2)-F(5)	149.23(15)
F(2)-Zr(1)-F(6)	73.51(13)	F(9)-Zr(2)-F(5)	89.82(14)
F(4)-Zr(1)-F(6)	76.08(15)	F(10)-Zr(2)-F(5)	137.24(13)
F(1)#1-Zr(1)-F(6)	139.60(14)	F(6)-Zr(2)-F(5)	66.60(13)
F(3)-Zr(1)-O(1)	96.04(18)	F(7)-Zr(2)-Zr(1)	89.34(12)
F(2)-Zr(1)-O(1)	148.29(16)	F(8)-Zr(2)-Zr(1)	107.57(11)
F(4)-Zr(1)-O(1)	90.05(17)	F(11)-Zr(2)-Zr(1)	176.09(13)
F(1)#1-Zr(1)-O(1)	77.05(16)	F(9)-Zr(2)-Zr(1)	92.34(11)
F(6)-Zr(1)-O(1)	137.33(16)	F(10)-Zr(2)-Zr(1)	103.91(10)
F(3)-Zr(1)-F(5)	76.76(16)	F(6)-Zr(2)-Zr(1)	32.72(9)
F(2)-Zr(1)-F(5)	138.20(13)	F(5)-Zr(2)-Zr(1)	33.89(9)
F(4)-Zr(1)-F(5)	75.94(14)	N(5)-Co(1)-N(1)	89.9(2)
F(1)#1-Zr(1)-F(5)	136.76(13)	N(5)-Co(1)-N(6)	85.3(2)
F(6)-Zr(1)-F(5)	64.76(12)	N(1)-Co(1)-N(6)	92.8(2)
O(1)-Zr(1)-F(5)	72.79(16)	N(5)-Co(1)-N(4)	92.9(2)
F(3)-Zr(1)-F(1)	140.01(15)	N(1)-Co(1)-N(4)	176.4(2)
F(2)-Zr(1)-F(1)	77.71(14)	N(6)-Co(1)-N(4)	89.7(2)
F(4)-Zr(1)-F(1)	70.93(13)	N(5)-Co(1)-N(2)	174.6(2)

F(1)#1-Zr(1)-F(1)	63.71(15)	N(1)-Co(1)-N(2)	85.6(2)
F(6)-Zr(1)-F(1)	134.78(13)	N(6)-Co(1)-N(2)	91.8(2)
O(1)-Zr(1)-F(1)	73.20(16)	N(4)-Co(1)-N(2)	91.7(2)
F(5)-Zr(1)-F(1)	131.77(13)	N(5)-Co(1)-N(3)	90.4(2)
F(3)-Zr(1)-Zr(2)	75.97(11)	N(1)-Co(1)-N(3)	92.0(2)
F(2)-Zr(1)-Zr(2)	105.43(10)	N(6)-Co(1)-N(3)	173.5(2)
F(4)-Zr(1)-Zr(2)	72.92(10)	N(4)-Co(1)-N(3)	85.6(2)
F(1)#1-Zr(1)-Zr(2)	152.38(10)	N(2)-Co(1)-N(3)	92.9(2)
F(6)-Zr(1)-Zr(2)	31.98(9)	Zr(1)#1-F(1)-Zr(1)	116.29(15)
O(1)-Zr(1)-Zr(2)	105.45(13)	Zr(2)-F(5)-Zr(1)	113.32(15)
F(5)-Zr(1)-Zr(2)	32.79(9)	Zr(2)-F(6)-Zr(1)	115.30(15)
F(1)-Zr(1)-Zr(2)	143.82(9)	C(2)-C(1)-N(1)	110.6(6)
F(7)-Zr(2)-F(8)	96.71(16)	C(1)-C(2)-N(2)	108.1(6)
F(7)-Zr(2)-F(11)	88.01(18)	N(3)-C(3)-C(4)	106.7(5)
F(8)-Zr(2)-F(11)	75.62(15)	N(4)-C(4)-C(3)	106.2(5)
F(7)-Zr(2)-F(9)	176.09(16)	N(5)-C(5)-C(6)	106.5(5)
F(8)-Zr(2)-F(9)	86.15(15)	N(6)-C(6)-C(5)	106.7(5)
F(11)-Zr(2)-F(9)	90.13(18)	C(1)-N(1)-Co(1)	109.6(4)
F(7)-Zr(2)-F(10)	91.67(16)	C(2)-N(2)-Co(1)	109.3(4)
F(8)-Zr(2)-F(10)	147.46(15)	C(3)-N(3)-Co(1)	108.1(4)
F(11)-Zr(2)-F(10)	73.31(15)	C(4)-N(4)-Co(1)	109.2(4)
F(9)-Zr(2)-F(10)	84.50(15)	C(5)-N(5)-Co(1)	110.1(4)
F(7)-Zr(2)-F(6)	86.22(16)	C(6)-N(6)-Co(1)	109.9(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1

Table S3

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1W)...F(10)#2	0.81(6)	1.72(6)	2.524(6)	171(6)
O(1)-H(2W)...F(2)#1	0.86(11)	1.76(11)	2.609(6)	171(10)
N(1)-H(1C)...F(9)#3	0.9	2.09	2.970(6)	166.6
N(1)-H(1D)...F(4)#4	0.9	2.28	3.028(6)	139.8
N(1)-H(1D)...F(7)#4	0.9	2.31	3.015(6)	134.7
N(2)-H(2C)...F(4)#5	0.9	2.24	3.095(7)	157.8
N(2)-H(2D)...F(9)#6	0.9	2.02	2.865(6)	155.6
N(3)-H(3D)...F(6)#4	0.9	2.13	3.005(6)	163.9
N(4)-H(4C)...F(11)	0.9	1.96	2.822(6)	159.5
N(4)-H(4D)...F(9)#6	0.9	2.32	3.134(6)	149.9
N(5)-H(5C)...F(11)	0.9	1.96	2.780(6)	150.5
N(5)-H(5D)...F(4)#4	0.9	2.13	2.980(6)	157.1
N(5)-H(5D)...F(2)#4	0.9	2.35	2.922(6)	121.3
N(6)-H(6C)...F(10)#3	0.9	1.88	2.736(6)	157.3
N(6)-H(6D)...F(8)#6	0.9	1.99	2.804(6)	149.6

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 x,-y+1/2,z+1/2 #3 -x+1,y+1/2,-z+1/2

#4 -x,y+1/2,-z+1/2 #5 -x,-y+1,-z+1 #6 -x+1,-y+1,-z+1