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Supporting Information

Self-Assembly of Linear [$Mn^{II}_2Mn^{III}$] Units with End-On Azido Bridges: The Construction of Ferromagnetic Chain using S_T = 7 High-Spin Trimers

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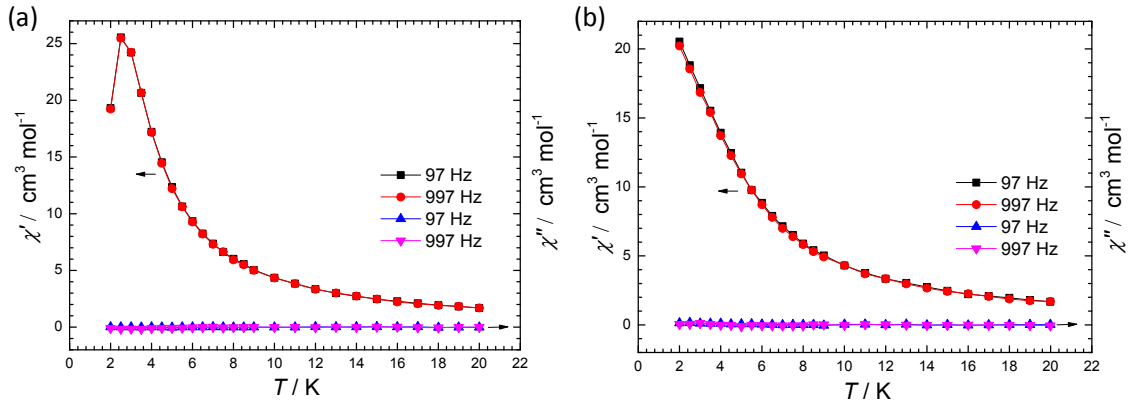

Figure **S1**: AC magnetic susceptibilities of compound **2** measured under 0 (a) and 1000 Oe (b) dc field, respectively.

Mn(1)-O(1)#1	1.890(4)
Mn(1)-O(1)	1.890(4)
Mn(1)-O(2)#1	1.902(3)
Mn(1)-O(2)	1.902(3)
Mn(1)-Br(1)	2.9151(9)
Mn(1)-Br(1)#1	2.9151(9)
Mn(1)-Mn(2)	3.2248(14)
Mn(1)-Mn(2)#1	3.2248(14)
Mn(2)-O(5)	2.173(4)
Mn(2)-O(3)	2.200(5)
Mn(2)-O(1)	2.206(3)
Mn(2)-O(2)#1	2.227(4)
Mn(2)-O(4)	2.232(5)
Mn(2)-Br(2)	2.5728(14)
O(1)-C(2)	1.423(6)
O(2)-C(3)	1.398(6)
O(2)-Mn(2)#1	2.227(4)
O(3)-C(17)	1.380(14)
O(3)-C(17')	1.447(14)
O(3)-H(3)	0.9300
O(4)-C(18)	1.391(10)
O(4)-H(4)	0.9300
O(5)-C(19)	1.408(8)
O(5)-H(5)	0.9300
N(1)-C(1)	1.494(6)
N(1)-C(4)	1.514(6)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
C(1)-C(3)	1.515(8)
C(1)-C(2)	1.539(7)
C(1)-H(1)	0.9800
C(2)-H(2A)	0.9700

C(2)-H(2B)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(16)	1.488(7)
C(4)-C(5)	1.525(7)
C(4)-H(4A)	0.9800
C(5)-C(6)	1.3900
C(5)-C(10)	1.3900
C(6)-C(7)	1.3900
C(6)-H(6)	0.9300
C(7)-C(8)	1.3900
C(7)-H(7)	0.9300
C(8)-C(9)	1.3900
C(8)-H(8)	0.9300
C(9)-C(10)	1.3900
C(9)-H(9)	0.9300
C(10)-C(11)	1.479(6)
C(11)-C(12)	1.3900
C(11)-C(16)	1.3900
C(12)-C(13)	1.3900
C(12)-H(12)	0.9300
C(13)-C(14)	1.3900
C(13)-H(13)	0.9300
C(14)-C(15)	1.3900
C(14)-H(14)	0.9300
C(15)-C(16)	1.3900
C(15)-H(15)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(17')-H(17D)	0.9600
C(17')-H(17E)	0.9600
C(17')-H(17F)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
O(6)-C(20')	1.321(16)
O(6)-C(20)	1.404(16)
O(6)-H(6A)	1.04(2)
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(20')-H(20D)	0.9600
C(20')-H(20E)	0.9600
C(20')-H(20F)	0.9600
O(1)#1-Mn(1)-O(1)	180.000(1)
O(1)#1-Mn(1)-O(2)#1	95.97(16)
O(1)-Mn(1)-O(2)#1	84.03(16)
O(1)#1-Mn(1)-O(2)	84.03(16)
O(1)-Mn(1)-O(2)	95.97(16)
O(2)#1-Mn(1)-O(2)	180.000(1)

O(1)#1-Mn(1)-Br(1)	89.00(11)
O(1)-Mn(1)-Br(1)	91.00(11)
O(2)#1-Mn(1)-Br(1)	87.45(10)
O(2)-Mn(1)-Br(1)	92.55(10)
O(1)#1-Mn(1)-Br(1)#1	91.00(11)
O(1)-Mn(1)-Br(1)#1	89.00(11)
O(2)#1-Mn(1)-Br(1)#1	92.55(10)
O(2)-Mn(1)-Br(1)#1	87.45(10)
Br(1)-Mn(1)-Br(1)#1	180.000(18)
O(1)#1-Mn(1)-Mn(2)	138.32(10)
O(1)-Mn(1)-Mn(2)	41.68(10)
O(2)#1-Mn(1)-Mn(2)	42.39(12)
O(2)-Mn(1)-Mn(2)	137.61(12)
Br(1)-Mn(1)-Mn(2)	90.44(3)
Br(1)#1-Mn(1)-Mn(2)	89.56(3)
O(1)#1-Mn(1)-Mn(2)#1	41.68(10)
O(1)-Mn(1)-Mn(2)#1	138.32(10)
O(2)#1-Mn(1)-Mn(2)#1	137.61(12)
O(2)-Mn(1)-Mn(2)#1	42.39(12)
Br(1)-Mn(1)-Mn(2)#1	89.56(3)
Br(1)#1-Mn(1)-Mn(2)#1	90.44(3)
Mn(2)-Mn(1)-Mn(2)#1	180.0
O(5)-Mn(2)-O(3)	88.55(19)
O(5)-Mn(2)-O(1)	164.48(18)
O(3)-Mn(2)-O(1)	87.33(16)
O(5)-Mn(2)-O(2)#1	94.92(17)
O(3)-Mn(2)-O(2)#1	85.72(18)
O(1)-Mn(2)-O(2)#1	69.85(14)
O(5)-Mn(2)-O(4)	88.09(19)
O(3)-Mn(2)-O(4)	167.6(2)
O(1)-Mn(2)-O(4)	92.76(15)
O(2)#1-Mn(2)-O(4)	82.67(17)
O(5)-Mn(2)-Br(2)	97.31(15)
O(3)-Mn(2)-Br(2)	99.19(16)
O(1)-Mn(2)-Br(2)	98.11(11)
O(2)#1-Mn(2)-Br(2)	166.91(9)
O(4)-Mn(2)-Br(2)	93.08(15)
O(5)-Mn(2)-Mn(1)	130.07(15)
O(3)-Mn(2)-Mn(1)	86.90(14)
O(1)-Mn(2)-Mn(1)	34.73(10)
O(2)#1-Mn(2)-Mn(1)	35.16(8)
O(4)-Mn(2)-Mn(1)	86.14(13)
Br(2)-Mn(2)-Mn(1)	132.48(4)
C(2)-O(1)-Mn(1)	121.9(3)
C(2)-O(1)-Mn(2)	128.2(3)
Mn(1)-O(1)-Mn(2)	103.59(15)
C(3)-O(2)-Mn(1)	124.4(3)
C(3)-O(2)-Mn(2)#1	126.6(3)
Mn(1)-O(2)-Mn(2)#1	102.45(16)
C(17)-O(3)-C(17')	23.6(10)
C(17)-O(3)-Mn(2)	140.8(9)
C(17')-O(3)-Mn(2)	120.4(8)
C(17)-O(3)-H(3)	109.6
C(17')-O(3)-H(3)	127.7
Mn(2)-O(3)-H(3)	109.6

C(18)-O(4)-Mn(2)	136.1(6)
C(18)-O(4)-H(4)	112.0
Mn(2)-O(4)-H(4)	112.0
C(19)-O(5)-Mn(2)	127.5(4)
C(19)-O(5)-H(5)	116.3
Mn(2)-O(5)-H(5)	116.3
C(1)-N(1)-C(4)	114.8(4)
C(1)-N(1)-H(1A)	108.6
C(4)-N(1)-H(1A)	108.6
C(1)-N(1)-H(1B)	108.6
C(4)-N(1)-H(1B)	108.6
H(1A)-N(1)-H(1B)	107.6
N(1)-C(1)-C(3)	111.2(5)
N(1)-C(1)-C(2)	108.9(4)
C(3)-C(1)-C(2)	113.2(4)
N(1)-C(1)-H(1)	107.8
C(3)-C(1)-H(1)	107.8
C(2)-C(1)-H(1)	107.8
O(1)-C(2)-C(1)	111.4(4)
O(1)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2A)	109.3
O(1)-C(2)-H(2B)	109.3
C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
O(2)-C(3)-C(1)	112.6(4)
O(2)-C(3)-H(3A)	109.1
C(1)-C(3)-H(3A)	109.1
O(2)-C(3)-H(3B)	109.1
C(1)-C(3)-H(3B)	109.1
H(3A)-C(3)-H(3B)	107.8
C(16)-C(4)-N(1)	111.9(4)
C(16)-C(4)-C(5)	103.0(4)
N(1)-C(4)-C(5)	111.3(5)
C(16)-C(4)-H(4A)	110.1
N(1)-C(4)-H(4A)	110.1
C(5)-C(4)-H(4A)	110.1
C(6)-C(5)-C(10)	120.0
C(6)-C(5)-C(4)	131.2(4)
C(10)-C(5)-C(4)	108.8(4)
C(7)-C(6)-C(5)	120.0
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	120.0
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-H(7)	120.0
C(9)-C(8)-C(7)	120.0
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	120.0
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(5)	120.0
C(9)-C(10)-C(11)	130.4(3)
C(5)-C(10)-C(11)	109.5(3)
C(12)-C(11)-C(16)	120.0

C(12)-C(11)-C(10)	132.7(3)
C(16)-C(11)-C(10)	107.3(3)
C(13)-C(12)-C(11)	120.0
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	120.0
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.0
C(13)-C(14)-H(14)	120.0
C(15)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	120.0
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(11)	120.0
C(15)-C(16)-C(4)	128.6(4)
C(11)-C(16)-C(4)	111.4(4)
O(3)-C(17)-H(17A)	109.5
O(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(3)-C(17')-H(17D)	109.5
O(3)-C(17')-H(17E)	109.5
H(17D)-C(17')-H(17E)	109.5
O(3)-C(17')-H(17F)	109.5
H(17D)-C(17')-H(17F)	109.5
H(17E)-C(17')-H(17F)	109.5
O(4)-C(18)-H(18A)	109.5
O(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(5)-C(19)-H(19A)	109.5
O(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(20')-O(6)-C(20)	29.2(13)
C(20')-O(6)-H(6A)	133(6)
C(20)-O(6)-H(6A)	120(6)
O(6)-C(20)-H(20A)	109.5
O(6)-C(20)-H(20B)	109.5
O(6)-C(20)-H(20C)	109.5
O(6)-C(20')-H(20D)	109.5
O(6)-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20E)	109.5
O(6)-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20F)	109.5
H(20E)-C(20')-H(20F)	109.5

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

Table S1: Detailed bond length and bond angles of **1**.

Mn(1)-O(2)	1.889(4)
Mn(1)-O(2)#1	1.889(4)
Mn(1)-O(1)#1	1.892(4)
Mn(1)-O(1)	1.892(4)
Mn(1)-Br(1)#1	2.9028(12)
Mn(1)-Br(1)	2.9028(12)
Mn(1)-Mn(2)#1	3.1962(13)
Mn(1)-Mn(2)	3.1962(13)
Mn(2)-O(1)	2.181(4)
Mn(2)-O(2)#1	2.187(5)
Mn(2)-O(3)	2.192(6)
Mn(2)-O(5)#2	2.283(7)
Mn(2)-N(2)#2	2.283(7)
Mn(2)-N(2)	2.340(7)
Mn(2)-Br(2)	2.6140(16)
O(1)-C(2)	1.440(8)
O(2)-C(3)	1.411(8)
O(2)-Mn(2)#1	2.187(5)
O(3)-C(17)	1.418(13)
O(3)-H(3)	0.9300
N(1)-C(1)	1.502(10)
N(1)-C(4)	1.546(9)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
N(2)-N(3)	1.181(13)
N(2)-Mn(2)#2	2.283(7)
N(3)-N(4)	1.131(14)
C(1)-C(3)	1.507(9)
C(1)-C(2)	1.514(9)
C(1)-H(1)	0.9800
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.486(11)
C(4)-C(16)	1.522(11)
C(4)-H(4)	0.9800
C(5)-C(6)	1.385(12)
C(5)-C(10)	1.417(10)
C(6)-C(7)	1.401(12)
C(6)-H(6)	0.9300
C(7)-C(8)	1.384(14)
C(7)-H(7)	0.9300
C(8)-C(9)	1.389(15)
C(8)-H(8)	0.9300
C(9)-C(10)	1.412(12)
C(9)-H(9)	0.9300
C(10)-C(11)	1.444(12)

C(11)-C(12)	1.376(11)
C(11)-C(16)	1.394(11)
C(12)-C(13)	1.379(14)
C(12)-H(12)	0.9300
C(13)-C(14)	1.373(14)
C(13)-H(13)	0.9300
C(14)-C(15)	1.338(13)
C(14)-H(14)	0.9300
C(15)-C(16)	1.401(13)
C(15)-H(15)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
O(4)-C(18)	1.41(3)
O(4)-H(4A)	0.8200
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
O(2)-Mn(1)-O(2)#1	180.00(19)
O(2)-Mn(1)-O(1)#1	83.45(18)
O(2)#1-Mn(1)-O(1)#1	96.55(18)
O(2)-Mn(1)-O(1)	96.55(18)
O(2)#1-Mn(1)-O(1)	83.45(18)
O(1)#1-Mn(1)-O(1)	180.0(3)
O(2)-Mn(1)-Br(1)#1	90.79(15)
O(2)#1-Mn(1)-Br(1)#1	89.21(15)
O(1)#1-Mn(1)-Br(1)#1	91.90(14)
O(1)-Mn(1)-Br(1)#1	88.10(14)
O(2)-Mn(1)-Br(1)	89.21(15)
O(2)#1-Mn(1)-Br(1)	90.79(15)
O(1)#1-Mn(1)-Br(1)	88.10(14)
O(1)-Mn(1)-Br(1)	91.90(14)
Br(1)#1-Mn(1)-Br(1)	180.0
O(2)-Mn(1)-Mn(2)#1	41.80(13)
O(2)#1-Mn(1)-Mn(2)#1	138.20(13)
O(1)#1-Mn(1)-Mn(2)#1	41.64(12)
O(1)-Mn(1)-Mn(2)#1	138.36(12)
Br(1)#1-Mn(1)-Mn(2)#1	91.85(3)
Br(1)-Mn(1)-Mn(2)#1	88.15(3)
O(2)-Mn(1)-Mn(2)	138.20(13)
O(2)#1-Mn(1)-Mn(2)	41.80(13)
O(1)#1-Mn(1)-Mn(2)	138.36(12)
O(1)-Mn(1)-Mn(2)	41.64(12)
Br(1)#1-Mn(1)-Mn(2)	88.15(3)
Br(1)-Mn(1)-Mn(2)	91.85(3)
Mn(2)#1-Mn(1)-Mn(2)	180.0
O(1)-Mn(2)-O(2)#1	70.34(16)
O(1)-Mn(2)-O(3)	94.19(19)
O(2)#1-Mn(2)-O(3)	85.3(2)
O(1)-Mn(2)-O(5)#2	97.3(2)
O(2)#1-Mn(2)-O(5)#2	87.9(2)
O(3)-Mn(2)-O(5)#2	163.9(2)
O(1)-Mn(2)-N(2)#2	97.3(2)
O(2)#1-Mn(2)-N(2)#2	87.9(2)

O(3)-Mn(2)-N(2)#2	163.9(2)
O(5)#2-Mn(2)-N(2)#2	0.0(4)
O(1)-Mn(2)-N(2)	163.4(2)
O(2)#1-Mn(2)-N(2)	93.38(19)
O(3)-Mn(2)-N(2)	87.2(2)
O(5)#2-Mn(2)-N(2)	78.6(3)
N(2)#2-Mn(2)-N(2)	78.6(3)
O(1)-Mn(2)-Br(2)	94.30(12)
O(2)#1-Mn(2)-Br(2)	164.50(12)
O(3)-Mn(2)-Br(2)	94.05(16)
O(5)#2-Mn(2)-Br(2)	96.34(16)
N(2)#2-Mn(2)-Br(2)	96.34(16)
N(2)-Mn(2)-Br(2)	102.07(17)
O(1)-Mn(2)-Mn(1)	35.19(11)
O(2)#1-Mn(2)-Mn(1)	35.15(11)
O(3)-Mn(2)-Mn(1)	89.66(15)
O(5)#2-Mn(2)-Mn(1)	93.20(18)
N(2)#2-Mn(2)-Mn(1)	93.20(18)
N(2)-Mn(2)-Mn(1)	128.47(17)
Br(2)-Mn(2)-Mn(1)	129.45(4)
C(2)-O(1)-Mn(1)	122.9(4)
C(2)-O(1)-Mn(2)	128.1(4)
Mn(1)-O(1)-Mn(2)	103.17(18)
C(3)-O(2)-Mn(1)	122.5(4)
C(3)-O(2)-Mn(2)#1	128.8(4)
Mn(1)-O(2)-Mn(2)#1	103.05(19)
C(17)-O(3)-Mn(2)	128.8(6)
C(17)-O(3)-H(3)	115.6
Mn(2)-O(3)-H(3)	115.6
C(1)-N(1)-C(4)	117.4(5)
C(1)-N(1)-H(1A)	108.0
C(4)-N(1)-H(1A)	108.0
C(1)-N(1)-H(1B)	108.0
C(4)-N(1)-H(1B)	108.0
H(1A)-N(1)-H(1B)	107.2
N(3)-N(2)-Mn(2)#2	122.9(7)
N(3)-N(2)-Mn(2)	121.7(6)
Mn(2)#2-N(2)-Mn(2)	101.4(3)
N(4)-N(3)-N(2)	173.4(14)
N(1)-C(1)-C(3)	108.4(5)
N(1)-C(1)-C(2)	112.6(6)
C(3)-C(1)-C(2)	113.2(6)
N(1)-C(1)-H(1)	107.5
C(3)-C(1)-H(1)	107.5
C(2)-C(1)-H(1)	107.5
O(1)-C(2)-C(1)	111.0(5)
O(1)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2A)	109.4
O(1)-C(2)-H(2B)	109.4
C(1)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
O(2)-C(3)-C(1)	113.1(6)
O(2)-C(3)-H(3A)	109.0
C(1)-C(3)-H(3A)	109.0
O(2)-C(3)-H(3B)	109.0

C(1)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
C(5)-C(4)-C(16)	102.9(6)
C(5)-C(4)-N(1)	112.8(6)
C(16)-C(4)-N(1)	107.5(6)
C(5)-C(4)-H(4)	111.1
C(16)-C(4)-H(4)	111.1
N(1)-C(4)-H(4)	111.1
C(6)-C(5)-C(10)	119.4(7)
C(6)-C(5)-C(4)	131.0(7)
C(10)-C(5)-C(4)	109.6(7)
C(5)-C(6)-C(7)	119.7(8)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-H(6)	120.1
C(8)-C(7)-C(6)	120.4(9)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	121.7(9)
C(7)-C(8)-H(8)	119.2
C(9)-C(8)-H(8)	119.2
C(8)-C(9)-C(10)	117.8(8)
C(8)-C(9)-H(9)	121.1
C(10)-C(9)-H(9)	121.1
C(9)-C(10)-C(5)	120.9(8)
C(9)-C(10)-C(11)	130.1(7)
C(5)-C(10)-C(11)	109.0(7)
C(12)-C(11)-C(16)	120.0(8)
C(12)-C(11)-C(10)	131.3(8)
C(16)-C(11)-C(10)	108.7(7)
C(11)-C(12)-C(13)	118.0(8)
C(11)-C(12)-H(12)	121.0
C(13)-C(12)-H(12)	121.0
C(14)-C(13)-C(12)	121.1(9)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(15)-C(14)-C(13)	122.5(10)
C(15)-C(14)-H(14)	118.7
C(13)-C(14)-H(14)	118.7
C(14)-C(15)-C(16)	117.3(9)
C(14)-C(15)-H(15)	121.3
C(16)-C(15)-H(15)	121.3
C(11)-C(16)-C(15)	121.1(8)
C(11)-C(16)-C(4)	109.7(8)
C(15)-C(16)-C(4)	129.2(7)
O(3)-C(17)-H(17A)	109.5
O(3)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(3)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(18)-O(4)-H(4A)	109.5
O(4)-C(18)-H(18A)	109.5
O(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(4)-C(18)-H(18C)	109.5

H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1 #2 -x+1,-y,-z+1

Table S2: Detailed bond length and bond angles of **2**.