

Supporting information

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Table S1. Bond lengths (Å) and angles (°) for(II)

Ni(1)-O(1)#1	2.0923(14)
Ni(1)-O(1)#2	2.0923(15)
Ni(1)-O(1)#3	2.0923(14)
Ni(1)-O(1)#4	2.0921(14)
Ni(1)-O(1)#5	2.0921(14)
Ni(1)-O(1)	2.0921(14)
Mn(1)-O(1)#1	2.0923(14)
Mn(1)-O(1)#2	2.0923(15)
Mn(1)-O(1)#5	2.0921(14)
Mn(1)-O(1)	2.0921(14)
Mn(1)-O(1)#3	2.0923(14)
Mn(1)-O(1)#4	2.0921(14)
S(1)-O(2)#6	1.474(4)
S(1)-O(2)#7	1.474(4)
S(1)-O(2)#8	1.474(4)
S(1)-O(2)#9	1.474(4)
S(1)-O(2)#10	1.474(4)
S(1)-O(2)	1.474(4)
S(1)-O(3)	1.323(13)
S(1)-O(3)#7	1.323(13)
O(1)-C(1)	1.256(3)
O(3)-O(2)#9	1.553(8)
O(3)-O(2)#7	1.553(8)
O(3)-O(2)#10	1.553(8)
N(1)-H(1)	0.8600
N(1)-C(1)	1.332(3)
N(1)-C(2)	1.441(4)
N(2)-H(2A)	0.8600
N(2)-H(2B)	0.8600
N(2)-C(1)	1.328(3)
C(2)-H(2C)	0.9600
C(2)-H(2D)	0.9600
C(2)-H(2E)	0.9600
O(1)#4-Ni(1)-O(1)#5	92.92(6)

O(1)#4-Ni(1)-O(1)#2	87.08(6)
O(1)#1-Ni(1)-O(1)#2	92.91(6)
O(1)#2-Ni(1)-O(1)#5	180.0
O(1)#4-Ni(1)-O(1)#3	179.990(1)
O(1)#4-Ni(1)-O(1)#1	87.08(6)
O(1)#5-Ni(1)-O(1)	92.92(6)
O(1)#1-Ni(1)-O(1)#5	87.08(6)
O(1)#1-Ni(1)-O(1)#3	92.91(6)
O(1)#2-Ni(1)-O(1)	87.08(6)
O(1)#5-Ni(1)-O(1)#3	87.08(6)
O(1)#4-Ni(1)-O(1)	92.92(6)
O(1)#1-Ni(1)-O(1)	179.99(9)
O(1)#2-Ni(1)-O(1)#3	92.91(6)
O(1)-Ni(1)-O(1)#3	87.08(6)
O(1)#4-Mn(1)-O(1)#1	87.08(6)
O(1)#4-Mn(1)-O(1)#3	179.990(1)
O(1)#1-Mn(1)-O(1)	179.99(9)
O(1)#5-Mn(1)-O(1)	92.92(6)
O(1)#1-Mn(1)-O(1)#2	92.91(6)
O(1)#2-Mn(1)-O(1)	87.08(6)
O(1)#1-Mn(1)-O(1)#5	87.08(6)
O(1)#2-Mn(1)-O(1)#3	92.91(6)
O(1)#2-Mn(1)-O(1)#5	180.0
O(1)#5-Mn(1)-O(1)#3	87.08(6)
O(1)#4-Mn(1)-O(1)	92.92(6)
O(1)#1-Mn(1)-O(1)#3	92.91(6)
O(1)#4-Mn(1)-O(1)#5	92.92(6)
O(1)#4-Mn(1)-O(1)#2	87.08(6)
O(1)-Mn(1)-O(1)#3	87.08(6)
O(2)#8-S(1)-O(2)#7	96.7(3)
O(2)-S(1)-O(2)#8	106.0(3)
O(2)-S(1)-O(2)#7	55.3(4)
O(2)#8-S(1)-O(2)#9	55.3(4)
O(2)#7-S(1)-O(2)#9	106.0(3)
O(2)-S(1)-O(2)#9	154.4(3)
O(3)#7-S(1)-O(2)#7	112.8(2)
O(3)-S(1)-O(2)#9	67.2(2)
O(3)#7-S(1)-O(2)	67.2(2)
O(3)#7-S(1)-O(2)#8	67.2(2)
O(3)-S(1)-O(2)#7	67.2(2)
O(3)-S(1)-O(2)#8	112.8(2)
O(3)#7-S(1)-O(2)#9	112.8(2)
O(3)-S(1)-O(2)	112.8(2)
O(3)#7-S(1)-O(3)	180.0

C(1)-O(1)-Ni(1)	128.21(15)
C(1)-O(1)-Mn(1)	128.21(15)
S(1)-O(3)-O(2)#9	61.0(4)
S(1)-O(3)-O(2)#7	61.0(4)
O(2)#7-O(3)-O(2)#9	98.5(6)
C(1)-N(1)-H(1)	118.5
C(1)-N(1)-C(2)	123.1(3)
C(2)-N(1)-H(1)	118.5
H(2A)-N(2)-H(2B)	120.0
C(1)-N(2)-H(2A)	120.0
C(1)-N(2)-H(2B)	120.0
O(1)-C(1)-N(1)	120.5(2)
O(1)-C(1)-N(2)	122.1(2)
N(2)-C(1)-N(1)	117.4(2)
N(1)-C(2)-H(2C)	109.5
N(1)-C(2)-H(2D)	109.5
N(1)-C(2)-H(2E)	109.5
H(2D)-C(2)-H(2C)	109.5
H(2D)-C(2)-H(2E)	109.5
H(2E)-C(2)-H(2C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3, -y + 2/3, -z + 2/3$ #2 $y + 1/3, -x + y + 2/3, -z + 2/3$
#3 $x - y + 1/3, x - 1/3, -z + 2/3$ #4 $-x + y + 1, -x + 1, z$ #5 $-y + 1, x - y, z$
#6 $-y + 1, x - y + 1, z$ #7 $y - 1/3, x + 1/3, -z + 5/6$ #8 $-x + y, -x + 1, z$
#9 $x - y + 2/3, -y + 4/3, -z + 5/6$ #10 $-x + 2/3, -x + y + 1/3, -z + 5/6$

Table S2. Torsion angles (°) for(II)

Ni(1)-O(1)-C(1)-N(1)	-145.9(2)
Ni(1)-O(1)-C(1)-N(2)	34.9(3)
Mn(1)-O(1)-C(1)-N(1)	-145.9(2)
Mn(1)-O(1)-C(1)-N(2)	34.9(3)
O(2)#8-S(1)-O(3)-O(2)#9	32.2(3)
O(2)-S(1)-O(3)-O(2)#9	152.2(3)
O(2)#7-S(1)-O(3)-O(2)#9	120.000(2)
O(2)#9-S(1)-O(3)-O(2)#7	-120.000(1)
O(2)#8-S(1)-O(3)-O(2)#7	-87.8(3)
O(2)-S(1)-O(3)-O(2)#7	32.2(3)
C(2)-N(1)-C(1)-O(1)	-5.0(5)
C(2)-N(1)-C(1)-N(2)	174.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3, -y + 2/3, -z + 2/3$ #2 $y + 1/3, -x + y + 2/3, -z + 2/3$

#3 $x - y + 1/3, x - 1/3, -z + 2/3$ #4 $-x + y + 1, -x + 1, z$ #5 $-y + 1, x - y, z$
 #6 $-y + 1, x - y + 1, z$ #7 $y - 1/3, x + 1/3, -z + 5/6$ #8 $-x + y, -x + 1, z$
 #9 $x - y + 2/3, -y + 4/3, -z + 5/6$ #10 $-x + 2/3, -x + y + 1/3, -z + 5/6$

Table S3. Bond lengths (Å) and angles (°) for(III)

Ni(1)-O(1)#1	2.1366(13)
Ni(1)-O(1)#2	2.1365(13)
Ni(1)-O(1)#3	2.1366(13)
Ni(1)-O(1)#4	2.1366(13)
Ni(1)-O(1)#5	2.1365(13)
Ni(1)-O(1)	2.1366(13)
Mn(1)-O(1)#1	2.1366(13)
Mn(1)-O(1)#2	2.1365(13)
Mn(1)-O(1)#5	2.1365(13)
Mn(1)-O(1)	2.1366(13)
Mn(1)-O(1)#3	2.1366(13)
Mn(1)-O(1)#4	2.1366(13)
S(1)-O(2)#6	1.481(3)
S(1)-O(2)#7	1.481(3)
S(1)-O(2)#8	1.481(3)
S(1)-O(2)#9	1.481(3)
S(1)-O(2)#10	1.481(3)
S(1)-O(2)	1.481(3)
S(1)-O(2)#10	1.481(3)
S(1)-O(3)	1.306(11)
S(1)-O(3)#7	1.306(11)
O(1)-C(1)	1.255(2)
O(2)-O(2)#9	1.404(10)
O(2)-O(3)#7	1.534(6)
O(3)-O(2)#9	1.534(6)
O(3)-O(2)#7	1.534(6)
O(3)-O(2)#10	1.534(6)
N(1)-H(1)	0.8600
N(1)-C(1)	1.329(3)
N(1)-C(2)	1.432(4)
N(2)-H(2A)	0.8600
N(2)-H(2B)	0.8600
N(2)-C(1)	1.335(3)
C(2)-H(2C)	0.9600
C(2)-H(2D)	0.9600
C(2)-H(2E)	0.9600
O(1)#1-Ni(1)-O(1)#3	92.72(6)

O(1)#5-Ni(1)-O(1)#4	92.72(6)
O(1)#5-Ni(1)-O(1)	92.72(6)
O(1)#2-Ni(1)-O(1)#4	87.28(6)
O(1)#3-Ni(1)-O(1)	87.28(6)
O(1)#2-Ni(1)-O(1)	87.28(6)
O(1)#1-Ni(1)-O(1)#5	87.28(6)
O(1)#1-Ni(1)-O(1)#2	92.72(6)
O(1)#3-Ni(1)-O(1)#5	87.28(6)
O(1)#1-Ni(1)-O(1)	180.0
O(1)#2-Ni(1)-O(1)#5	180.0
O(1)#3-Ni(1)-O(1)#2	92.72(6)
O(1)#1-Ni(1)-O(1)#4	87.28(6)
O(1)#3-Ni(1)-O(1)#4	180.00(7)
O(1)#4-Ni(1)-O(1)	92.72(6)
O(1)#1-Mn(1)-O(1)#3	92.72(6)
O(1)#3-Mn(1)-O(1)#5	87.28(6)
O(1)#1-Mn(1)-O(1)#4	87.28(6)
O(1)#2-Mn(1)-O(1)#4	87.28(6)
O(1)#2-Mn(1)-O(1)#5	180.0
O(1)#5-Mn(1)-O(1)	92.72(6)
O(1)#5-Mn(1)-O(1)#4	92.72(6)
O(1)#1-Mn(1)-O(1)#2	92.72(6)
O(1)#3-Mn(1)-O(1)	87.28(6)
O(1)#1-Mn(1)-O(1)	180.0
O(1)#4-Mn(1)-O(1)	92.72(6)
O(1)#3-Mn(1)-O(1)#2	92.72(6)
O(1)#2-Mn(1)-O(1)	87.28(6)
O(1)#1-Mn(1)-O(1)#5	87.28(6)
O(1)#3-Mn(1)-O(1)#4	180.00(7)
O(2)#6-S(1)-O(2)#8	105.1(3)
O(2)#7-S(1)-O(2)#10	105.1(3)
O(2)#6-S(1)-O(2)#10	154.6(3)
O(2)-S(1)-O(2)#10	97.3(3)
O(2)#8-S(1)-O(2)#9	154.6(3)
O(2)-S(1)-O(2)#9	56.6(4)
O(2)#6-S(1)-O(2)#7	56.6(4)
O(2)#6-S(1)-O(2)	105.1(3)
O(2)#8-S(1)-O(2)#7	97.3(3)
O(2)#6-S(1)-O(2)#9	97.3(3)
O(2)#7-S(1)-O(2)#9	105.1(3)
O(2)#8-S(1)-O(2)	105.1(3)
O(2)-S(1)-O(2)#7	154.6(3)
O(2)#8-S(1)-O(2)#10	56.6(4)
O(2)#10-S(1)-O(2)#9	105.1(3)

O(3)-S(1)-O(2)	113.6(2)
O(3)#7-S(1)-O(2)#10	113.6(2)
O(3)#7-S(1)-O(2)#6	66.4(2)
O(3)#7-S(1)-O(2)	66.4(2)
O(3)-S(1)-O(2)#7	66.4(2)
O(3)-S(1)-O(2)#8	113.6(2)
O(3)#7-S(1)-O(2)#7	113.6(2)
O(3)-S(1)-O(2)#6	113.6(2)
O(3)-S(1)-O(2)#9	66.4(2)
O(3)-S(1)-O(2)#10	66.4(2)
O(3)#7-S(1)-O(2)#8	66.4(2)
O(3)#7-S(1)-O(2)#9	113.6(2)
O(3)#7-S(1)-O(3)	180.0
C(1)-O(1)-Ni(1)	128.07(13)
C(1)-O(1)-Mn(1)	128.07(13)
S(1)-O(2)-O(3)#7	51.3(4)
O(2)#9-O(2)-S(1)	61.7(2)
O(2)#9-O(2)-O(3)#7	105.1(4)
S(1)-O(3)-O(2)#7	62.3(4)
S(1)-O(3)-O(2)#10	62.3(4)
S(1)-O(3)-O(2)#9	62.3(4)
O(2)#10-O(3)-O(2)#9	100.1(5)
O(2)#7-O(3)-O(2)#9	100.1(5)
O(2)#10-O(3)-O(2)#7	100.1(5)
C(1)-N(1)-H(1)	118.4
C(1)-N(1)-C(2)	123.1(2)
C(2)-N(1)-H(1)	118.4
H(2A)-N(2)-H(2B)	120.0
C(1)-N(2)-H(2A)	120.0
C(1)-N(2)-H(2B)	120.0
O(1)-C(1)-N(1)	120.8(2)
O(1)-C(1)-N(2)	121.64(19)
N(1)-C(1)-N(2)	117.6(2)
N(1)-C(2)-H(2C)	109.5
N(1)-C(2)-H(2D)	109.5
N(1)-C(2)-H(2E)	109.5
H(2C)-C(2)-H(2D)	109.5
H(2C)-C(2)-H(2E)	109.5
H(2D)-C(2)-H(2E)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3, -y + 2/3, -z + 2/3$ #2 $y + 1/3, -x + y + 2/3, -z + 2/3$
#3 $x - y + 1/3, x - 1/3, -z + 2/3$ #4 $-x + y + 1, -x + 1, z$ #5 $-y + 1, x - y, z$
#6 $-y + 1, x - y + 1, z$ #7 $y - 1/3, x + 1/3, -z + 5/6$ #8 $-x + y, -x + 1, z$

#9 $x - y + 2/3$, $-y + 4/3$, $-z + 5/6$ #10 $-x + 2/3$, $-x + y + 1/3$, $-z + 5/6$

Table S4. Torsion angles (°) for(III)

Ni(1)-O(1)-C(1)-N(1)	144.76(19)
Ni(1)-O(1)-C(1)-N(2)	-36.2(3)
Mn(1)-O(1)-C(1)-N(1)	144.76(19)
Mn(1)-O(1)-C(1)-N(2)	-36.2(3)
O(2)#10-S(1)-O(2)-O(2)#9	103.3(4)
O(2)#6-S(1)-O(2)-O(2)#9	-88.8(5)
O(2)#8-S(1)-O(2)-O(2)#9	160.6(2)
O(2)#7-S(1)-O(2)-O(2)#9	-48.5(3)
O(2)#9-S(1)-O(2)-O(3)#7	144.1(3)
O(2)#7-S(1)-O(2)-O(3)#7	95.63(7)
O(2)#6-S(1)-O(2)-O(3)#7	55.3(2)
O(2)#8-S(1)-O(2)-O(3)#7	-55.3(2)
O(2)#10-S(1)-O(2)-O(3)#7	-112.6(2)
O(2)#9-S(1)-O(3)-O(2)#10	120.000(1)
O(2)#10-S(1)-O(3)-O(2)#7	120.001(4)
O(2)#6-S(1)-O(3)-O(2)#7	-32.3(3)
O(2)#9-S(1)-O(3)-O(2)#7	-119.999(3)
O(2)#6-S(1)-O(3)-O(2)#9	87.7(3)
O(2)#10-S(1)-O(3)-O(2)#9	-120.000(1)
O(2)#8-S(1)-O(3)-O(2)#10	-32.3(3)
O(2)-S(1)-O(3)-O(2)#9	-32.3(3)
O(2)-S(1)-O(3)-O(2)#10	87.7(3)
O(2)-S(1)-O(3)-O(2)#7	-152.3(3)
O(2)#7-S(1)-O(3)-O(2)#10	-120.001(1)
O(2)#8-S(1)-O(3)-O(2)#9	-152.3(3)
O(2)#7-S(1)-O(3)-O(2)#9	119.999(1)
O(2)#6-S(1)-O(3)-O(2)#10	-152.3(3)
O(2)#8-S(1)-O(3)-O(2)#7	87.7(3)
O(3)#7-S(1)-O(2)-O(2)#9	-144.1(3)
O(3)-S(1)-O(2)-O(2)#9	35.9(3)
O(3)-S(1)-O(2)-O(3)#7	180.000(4)
C(2)-N(1)-C(1)-O(1)	4.2(4)
C(2)-N(1)-C(1)-N(2)	-174.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3$, $-y + 2/3$, $-z + 2/3$ #2 $y + 1/3$, $-x + y + 2/3$, $-z + 2/3$
 #3 $x - y + 1/3$, $x - 1/3$, $-z + 2/3$ #4 $-x + y + 1$, $-x + 1$, z #5 $-y + 1$, $x - y$, z
 #6 $-y + 1$, $x - y + 1$, z #7 $y - 1/3$, $x + 1/3$, $-z + 5/6$ #8 $-x + y$, $-x + 1$, z
 #9 $x - y + 2/3$, $-y + 4/3$, $-z + 5/6$ #10 $-x + 2/3$, $-x + y + 1/3$, $-z + 5/6$

Table S5. Bond lengths (Å) and angles (°) for(IV).

Ni(1)-O(1)#1	2.1708(14)
Ni(1)-O(1)#2	2.1708(14)
Ni(1)-O(1)#3	2.1708(14)
Ni(1)-O(1)#4	2.1706(14)
Ni(1)-O(1)#5	2.1706(14)
Ni(1)-O(1)	2.1706(14)
Mn(1)-O(1)#1	2.1708(14)
Mn(1)-O(1)#2	2.1708(14)
Mn(1)-O(1)#5	2.1706(14)
Mn(1)-O(1)	2.1706(14)
Mn(1)-O(1)#3	2.1708(14)
Mn(1)-O(1)#4	2.1706(14)
S(1)-O(2)#6	1.485(3)
S(1)-O(2)#7	1.485(3)
S(1)-O(2)#8	1.485(3)
S(1)-O(2)#9	1.485(3)
S(1)-O(2)#10	1.485(3)
S(1)-O(2)	1.485(3)
S(1)-O(3)	1.291(11)
S(1)-O(3)#7	1.291(11)
O(1)-C(1)	1.258(2)
O(3)-O(2)#9	1.531(6)
O(3)-O(2)#7	1.531(6)
O(3)-O(2)#10	1.531(6)
N(1)-H(1)	0.8600
N(1)-C(1)	1.332(3)
N(1)-C(2)	1.439(4)
N(2)-H(2A)	0.8600
N(2)-H(2B)	0.8600
N(2)-C(1)	1.333(3)
C(2)-H(2C)	0.9600
C(2)-H(2D)	0.9600
C(2)-H(2E)	0.9600
O(1)#1-Ni(1)-O(1)#3	92.47(6)
O(1)#5-Ni(1)-O(1)#4	92.48(6)
O(1)#5-Ni(1)-O(1)	92.48(6)
O(1)#4-Ni(1)-O(1)#2	87.52(6)
O(1)#3-Ni(1)-O(1)	87.52(6)
O(1)#2-Ni(1)-O(1)	87.52(6)
O(1)#5-Ni(1)-O(1)#1	87.52(6)
O(1)#1-Ni(1)-O(1)#2	92.47(6)

O(1)#5-Ni(1)-O(1)#3	87.52(6)
O(1)#1-Ni(1)-O(1)	180.0
O(1)#5-Ni(1)-O(1)#2	180.0
O(1)#3-Ni(1)-O(1)#2	92.47(6)
O(1)#1-Ni(1)-O(1)#4	87.52(6)
O(1)#3-Ni(1)-O(1)#4	180.0
O(1)#4-Ni(1)-O(1)	92.48(6)
O(1)#5-Mn(1)-O(1)#1	87.52(6)
O(1)#3-Mn(1)-O(1)#2	92.47(6)
O(1)#3-Mn(1)-O(1)	87.52(6)
O(1)#5-Mn(1)-O(1)#3	87.52(6)
O(1)#5-Mn(1)-O(1)	92.48(6)
O(1)#1-Mn(1)-O(1)#3	92.47(6)
O(1)#1-Mn(1)-O(1)#2	92.47(6)
O(1)#5-Mn(1)-O(1)#4	92.48(6)
O(1)#4-Mn(1)-O(1)#2	87.52(6)
O(1)#1-Mn(1)-O(1)#4	87.52(6)
O(1)#1-Mn(1)-O(1)	180.0
O(1)#3-Mn(1)-O(1)#4	180.0
O(1)#2-Mn(1)-O(1)	87.52(6)
O(1)#5-Mn(1)-O(1)#2	180.0
O(1)#4-Mn(1)-O(1)	92.48(6)
C(1)-O(1)-Ni(1)	127.71(13)
C(1)-O(1)-Mn(1)	127.71(13)
C(1)-N(1)-H(1)	118.5
C(1)-N(1)-C(2)	122.9(2)
C(2)-N(1)-H(1)	118.5
H(2A)-N(2)-H(2B)	120.0
C(1)-N(2)-H(2A)	120.0
C(1)-N(2)-H(2B)	120.0
O(1)-C(1)-N(1)	120.8(2)
O(1)-C(1)-N(2)	121.7(2)
N(1)-C(1)-N(2)	117.5(2)
N(1)-C(2)-H(2C)	109.5
N(1)-C(2)-H(2D)	109.5
N(1)-C(2)-H(2E)	109.5
H(2C)-C(2)-H(2D)	109.5
H(2C)-C(2)-H(2E)	109.5
H(2D)-C(2)-H(2E)	109.5
O(2)#10-S(1)-O(2)#6	56.3(4)
O(2)#10-S(1)-O(2)	97.4(3)
O(2)-S(1)-O(2)#6	105.2(3)
O(3)#7-S(1)-O(2)#10	113.5(2)
O(3)#7-S(1)-O(2)#6	66.5(2)

O(3)-S(1)-O(2)#6	113.5(2)
O(3)-S(1)-O(2)#10	66.5(2)
O(3)-S(1)-O(2)	113.5(2)
O(3)#7-S(1)-O(2)	66.5(2)
O(3)-S(1)-O(3)#7	180.0
S(1)-O(3)-O(2)#10	62.8(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3, -y + 2/3, -z + 2/3$ #2 $y + 1/3, -x + y + 2/3, -z + 2/3$
 #3 $x - y + 1/3, x - 1/3, -z + 2/3$ #4 $-x + y + 1, -x + 1, z$ #5 $-y + 1, x - y, z$
 #6 $-y + 1, x - y + 1, z$ #7 $y - 1/3, x + 1/3, -z + 5/6$ #8 $-x + y, -x + 1, z$
 #9 $x - y + 2/3, -y + 4/3, -z + 5/6$ #10 $-x + 2/3, -x + y + 1/3, -z + 5/6$

Table S6. Torsion angles (°) for(IV).

Ni(1)-O(1)-C(1)-N(1)	143.9(2)
Ni(1)-O(1)-C(1)-N(2)	-37.1(3)
Mn(1)-O(1)-C(1)-N(1)	143.9(2)
Mn(1)-O(1)-C(1)-N(2)	-37.1(3)
C(2)-N(1)-C(1)-O(1)	4.1(4)
C(2)-N(1)-C(1)-N(2)	-174.9(3)
O(2)-S(1)-O(3)-O(2)#10	88.0(3)
O(2)#6-S(1)-O(3)-O(2)#10	-32.0(3)

Symmetry transformations used to generate equivalent atoms:

#1 $-x + 4/3, -y + 2/3, -z + 2/3$ #2 $y + 1/3, -x + y + 2/3, -z + 2/3$
 #3 $x - y + 1/3, x - 1/3, -z + 2/3$ #4 $-x + y + 1, -x + 1, z$ #5 $-y + 1, x - y, z$
 #6 $-y + 1, x - y + 1, z$ #7 $y - 1/3, x + 1/3, -z + 5/6$ #8 $-x + y, -x + 1, z$
 #9 $x - y + 2/3, -y + 4/3, -z + 5/6$ #10 $-x + 2/3, -x + y + 1/3, -z + 5/6$