Supplementary Materials

Red and *Blue-Black* Tin Monoxide, SnO: Pitfalls, Challenges, and Helpful Tools in Crystal Structure Determination of Low-Intensity Datasets from Microcrystals

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Table S1. Atomic coordinates of black-blue SnO at ambient temperature.

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for black-blue SnO at ambient temperature. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	2500	2500	2375(1)	11(1)
O(1)	7500	2500	0	13(1)

Table S2. Bond lengths and angles of black-blue SnO at ambient temperature.

Bond lengths [Å] and angles [°] for black-blue SnO at ambient temperature.

Sn(1)-O(1)#1	2.2213(1)
Sn(1)-O(1)#2	2.2213(1)
Sn(1)-O(1)#3	2.2213(1)
Sn(1)-O(1)	2.2213(1)
O(1)#1-Sn(1)-O(1)#2	74.48(1)
O(1)#1-Sn(1)-O(1)#3	117.71(1)
O(1)#2-Sn(1)-O(1)#3	74.48(1)
O(1)#1-Sn(1)-O(1)	74.48(1)
O(1)#2-Sn(1)-O(1)	117.71(1)
O(1)#3-Sn(1)-O(1)	74.48(1)
Sn(1)#1-O(1)-Sn(1)#4	105.52(1)
Sn(1)#1-O(1)-Sn(1)#3	117.71(1)
Sn(1)#4-O(1)-Sn(1)#3	105.52(1)
Sn(1)#1-O(1)-Sn(1)	105.52(1)
Sn(1)#4-O(1)-Sn(1)	117.71(1)
Sn(1)#3-O(1)-Sn(1)	105.52(1)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z   #2 x-1,y,z   #3 -x+1,-y+1,-z
#4 x+1,y,z

Table S3. Anisotropic thermal displacement parameters of black-blue SnO at ambient temperature.

Anisotropic displacement parameters (Å^2 x 10^3) for black-blue SnO at ambient temperature. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U11	U22	U33	U23	U13	U12
Sn(1)	11(1)	11(1)	12(1)	0	0	0
O(1)	11(1)	11(1)	18(1)	0	0	0

Table S4. Atomic coordinates of black-blue SnO at 100 K.

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for black-blue SnO at 100 K. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	2500	2500	2380(1)	4(1)
O(1)	7500	2500	0	5(1)

Table S5. Bond lengths and angles of black-blue SnO at 100 K.

Bond lengths [Å] and angles [°] for black-blue SnO at 100 K.

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```
    Sn(1)-O(1)#1                   2.2213(1)
    Sn(1)-O(1)#2                    2.2213(1)
    Sn(1)-O(1)#3                    2.2213(1)
    Sn(1)-O(1)                      2.2213(1)


    O(1)#1-Sn(1)-O(1)#2             74.48(1)
    O(1)#1-Sn(1)-O(1)#3            117.71(1)
    O(1)#2-Sn(1)-O(1)#3             74.48(1)
    O(1)#1-Sn(1)-O(1)              74.48(1)
    O(1)#2-Sn(1)-O(1)             117.71(1)
    O(1)#3-Sn(1)-O(1)              74.48(1)

    Sn(1)#1-O(1)-Sn(1)#4          105.52(1)
    Sn(1)#1-O(1)-Sn(1)#3          117.71(1)
    Sn(1)#4-O(1)-Sn(1)#3          105.52(1)
    Sn(1)#1-O(1)-Sn(1)            105.52(1)
    Sn(1)#4-O(1)-Sn(1)            117.71(1)
    Sn(1)#3-O(1)-Sn(1)            105.52(1)
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    Symmetry transformations used to generate equivalent atoms:
    #1 -x+1,-y,-z    #2 x-1,y,z    #3 -x+1,-y+1,-z
    #4 x+1,y,z
```

Table S6. Anisotropic thermal displacement parameters of black-blue SnO at 100 K.

Anisotropic displacement parameters (Å^2 x 10^3) for black-blue SnO at 100 K.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

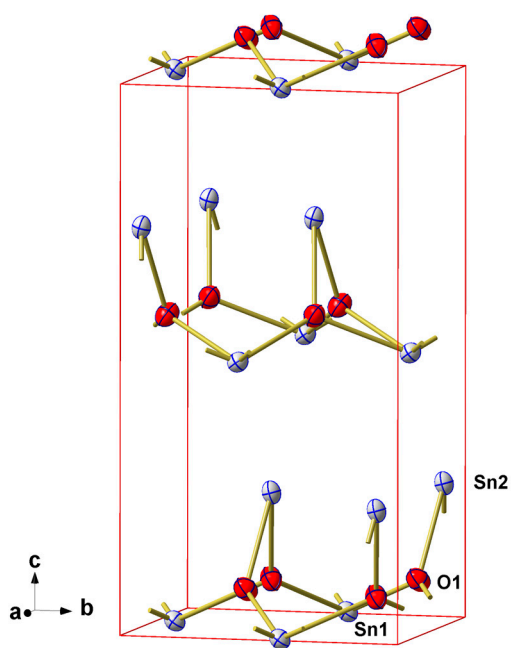|	U11	U22	U33	U23	U13	U12
Sn(1)	4(1)	4(1)	4(1)	0	0	0
O(1)	4(1)	4(1)	8(1)	0	0	0

Figure S1. Unit cell of red SnO in *Cmc2*$_1$.

Table S7. Crystallographic data or red SnO in *Cmc*2₁

```
Empirical formula               O Sn
Formula weight                  134.69
Temperature                     296(2) K
Wavelength                      0.71073 Å

Crystal system, space group     Orthorhombic, Cmc2₁
Unit cell dimensions            a =   5.0116(3) Å
                                b =   5.7445(4) Å
                                c =  11.0600(6) Å
Volume                          318.41(3) Å³
Z, Calculated density           8, 5.619 Mg/m^3
Absorption coefficient          15.433 mm^-1
F(000)                          464

Crystal size                    0.015 x 0.015 x 0.015 mm
Theta range for data collection 3.684 to 28.979 deg.
Limiting indices                -6<=h<=6, -7<=k<=7, -15<=l<=15
Reflections collected / unique  14367 / 466 [R(int) = 0.0591]
Completeness to theta = 25.242  100.0 %
Absorption correction           Semi-empirical from equivalents
Max. and min. transmission      0.813 and 0.674

Refinement method               Full-matrix least-squares on F^2
Data / restraints / parameters  466 / 1 / 23
Goodness-of-fit on F^2          1.225
Final R indices [I>2sigma(I)]   R1 = 0.0296, wR2 = 0.0698
R indices (all data)            R1 = 0.0339, wR2 = 0.0758
Absolute structure parameter    0.5(4)
Extinction coefficient          n/a
Largest diff. peak and hole     2.622 and -1.264 e.A^-3
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Table S8. Atomic coordinates of red SnO in *Cmc2₁* .

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for red SnO. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	0	5761(3)	27(1)	21(1)
Sn(2)	0	9238(3)	2414(1)	22(1)
O(1)	1870(20)	8770(20)	747(10)	30(2)

Table S9. Bond lengths and angles of red SnO in *Cmc2₁*.

```
Bond lengths [Å] and angles [°] for red SnO in Cmc2₁.
        Sn(1)-O(1)#1                2.098(12)
        Sn(1)-O(1)#2                2.098(12)
        Sn(1)-O(1)#3                2.121(11)
        Sn(1)-O(1)                  2.121(11)

        Sn(2)-O(1)#3                2.087(11)
        Sn(2)-O(1)                  2.087(11)


        O(1)#1-Sn(1)-O(1)#2          96.6(7)
        O(1)#1-Sn(1)-O(1)#3          88.4(3)
        O(1)#2-Sn(1)-O(1)#3         129.3(6)
        O(1)#1-Sn(1)-O(1)          129.3(6)
        O(1)#2-Sn(1)-O(1)           88.4(3)
        O(1)#3-Sn(1)-O(1)           52.6(7)

        O(1)#3-Sn(2)-O(1)           53.5(7)

        Sn(2)-O(1)-Sn(1)#4         126.9(6)
        Sn(2)-O(1)-Sn(1)          103.8(5)
        Sn(1)#4-O(1)-Sn(1)        129.3(6)
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        Symmetry transformations used to generate equivalent atoms:
        #1 x-1/2,y-1/2,z    #2 -x+1/2,y-1/2,z
        #3 -x,y,z    #4 x+1/2,y+1/2,z
```

Table S10. Anisotropic thermal displacement parameters of red SnO in *Cmc*2$_1$.

Anisotropic displacement parameters (Å^2 x 10^3) for red SnO in *Cmc*2$_1$.
The anisotropic displacement factor exponent takes the form:
-2π^2[h^{2}a*^{2}U$_{11}$ + ... + 2hka*b*U$_{12}$]

	U11	U22	U33	U23	U13	U12
Sn(1)	4(1)	4(1)	4(1)	0	0	0
O(1)	4(1)	4(1)	8(1)	0	0	0

Table S11. Atomic coordinates of red SnO in *Pbca*.

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for red SnO in Pbca. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	5084(1)	8262(1)	3806(1)	21(1)
O(1)	8107(9)	6264(9)	4519(5)	25(1)

Table S12. Bond lengths and angles of red SnO in *Pbca*.

Bond lengths [Å] and angles [°] for red SnO in Pbca.

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  Sn(1)-O(1)                     2.057(5)
  Sn(1)-O(1)#1                    2.102(5)
  Sn(1)-O(1)#2                    2.118(5)

  O(1)-Sn(1)-O(1)#1              89.8(1)
  O(1)-Sn(1)-O(1)#2             94.6(1)
  O(1)#1-Sn(1)-O(1)#2           76.6(2)

  Sn(1)-O(1)-Sn(1)#3           129.1(2)
  Sn(1)-O(1)-Sn(1)#4           127.4(2)
  Sn(1)#3-O(1)-Sn(1)#4         103.4(2)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,y+1/2,z     #2 x-1/2,-y+3/2,-z+1
#3 -x+3/2,y-1/2,z     #4 x+1/2,-y+3/2,-z+1
```

Table S13. Anisotropic thermal displacement parameters of red SnO in *Pbca*.

Anisotropic displacement parameters (Å^2 x 10^3) for red SnO in Pbca.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U11	U22	U33	U23	U13	U12
Sn(1)	17(1)	21(1)	24(1)	-2(1)	-3(1)	0(1)
O(1)	19(2)	23(2)	33(3)	-5(2)	-5(2)	5(2)