

Supplementary Information for

“Spin-orbit coupling induced semi-metallic state in the 1/3 hole-doped hyper-kagome Na₃Ir₃O₈”

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Structure Determination

Diffraction data were collected at 294 K on a three circle diffractometer (Bruker AXS, Karlsruhe, Germany) equipped with SMART APEX II CCD, using Mo- $K\alpha$ radiation ($\lambda = 0.71073$ Å). The collection and reduction of data were carried out with the BRUKER SUITE software package [S1]. The intensities were corrected for absorption effects applying a multi-scan method with SADABS [S2]. The structure was solved by Direct Methods and refined by full matrix least-squares fitting with the SHELXTL software package [S3]. The structure was refined as a two-component inversion twin with twin volume fractions close to racemic twinning (0.51(5)/0.49). Experimental details of data collection and crystallographic data are given in Table S1 and S2.

Supplementary Table S1: Crystal data and structure refinement data of Na₃Ir₃O₈.

	Na ₃ Ir ₃ O ₈
Temperature /K	294(2)
Formula weight	773.57
Space group (no.), <i>Z</i>	<i>P</i> 4 ₁ 32 (213), 4
Lattice constants /Å	<i>a</i> = 8.9857(4)
<i>V</i> /Å ³ , ρ_{xray} /g cm ⁻³	725.5(1), 7.082
Crystal size /mm ⁻³	0.08×0.06×0.04
Diffractometer	SMART APEX II, Bruker AXS
X-ray radiation, λ /Å	0.71073
Absorption correction	Multi-scan, SADABS ^[S2]
2 θ range /°	6.4-72.6
Index range	-14 ≤ <i>h</i> ≤ 14 -14 ≤ <i>k</i> ≤ 14 -14 ≤ <i>l</i> ≤ 14
Reflection collected	13526
Data, <i>R</i> _{int}	593, 0.045
No. of parameters	24
Transmission: <i>t</i> _{max} , <i>t</i> _{min}	0.166, 0.073
<i>R</i> 1 [<i>F</i> ² > 2σ(<i>F</i> ²)]	0.012
<i>wR</i> (<i>F</i> ²)	0.029
Absolute structure parameter	0.51(5)
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ /e Å ⁻³	0.893, -0.606
Deposition no. ^[S4]	CSD-426992

Supplementary Table S2. Atomic coordinates and displacement parameters $U_{ij}/\text{\AA}^2 \times 10^4$ for $\text{Na}_3\text{Ir}_3\text{O}_8$ at 294 K.

Atom	site	x	y	z
Ir	12d	0.61264(2)	$x + 1/4$	5/8
Na1	4b	7/8	7/8	7/8
Na2	8c	0.2570(2)	x	x
O1	8c	0.1144(3)	x	x
O2	24e	0.1364(3)	0.9071(3)	0.9186(3)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	U_{eq}
Ir	78.56(6)	U_{11}	83.5(8)	4.1(5)	-2.3(4)	$-U_{13}$	80.2(5)
Na1	122(6)	U_{11}	U_{11}	-18(8)	U_{12}	U_{12}	122(6)
Na2	138(5)	U_{11}	U_{11}	-2(6)	U_{12}	U_{12}	138(5)
O1	105(7)	U_{11}	U_{11}	2(9)	U_{12}	U_{12}	105(7)
O2	146(12)	103(11)	84(10)	-2(9)	13(9)	-1(8)	111(5)

Supplementary References:

[S1] *Bruker Suite*, Version 2008/3, Bruker AXS Inc., Madison USA **2008**.

[S2] G. M. Sheldrick, SADABS — *Bruker AXS area detector scaling and absorption*, Version 2008/1, University of Gottingen, Germany **2008**.

[S3] G. M. Sheldrick, *Acta Crystallogr., Sect. A* **2008**, *64*, 112-122.

[S4] Further details may be obtained from Fachinformationszentrum Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany (fax: (+49)-7247-808-666; e-mail: crysdata(at)fiz-karlsruhe.de, [http://www.fiz-karlsruhe.de/request for deposited data.html](http://www.fiz-karlsruhe.de/request%20for%20deposited%20data.html)) on quoting the CSD number (426992).