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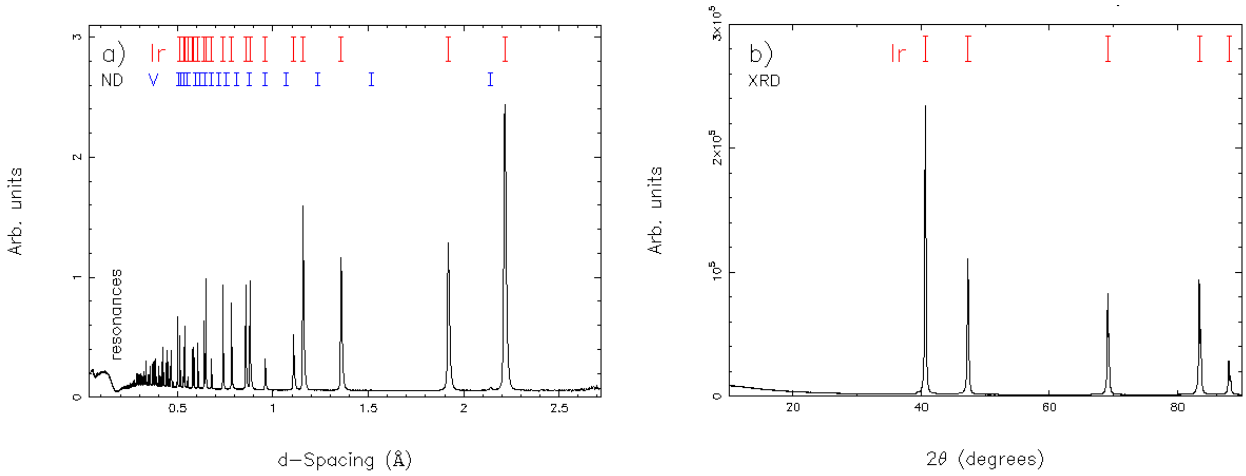

Figure S1 Diffraction patterns of ^{iso}Ir. a) Neutron diffraction measured by Bank5 of the GEM diffractometer (Hannon, 2005) with the sample inside a vanadium can. The tickmarks indicate the d-spacings of the predicted reflections of iridium (red) and vanadium (blue) that are longer than 0.5 Å. b) X-ray diffraction measured in flat-plate reflection geometry on a Rigaku MiniFlex 600 X-ray diffractometer with a copper anode. All of the observed reflections are consistent with the ^{iso}Ir being metallic iridium (FCC, a=3.8394 Å (Swanson *et al.*, 1955)), and indicate that the isotopically enriched metal powder was chemically pure.

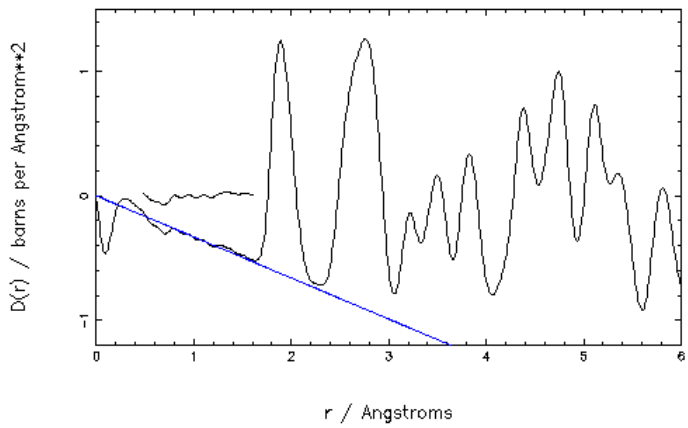

Figure S2 The experimental differential correlation function, $D_{exp}(r)$, for Al_2O_3 (black continuous line). a) Also shown is the fit (blue) to the experimental data over the distance range 0.50 Å to 1.60 Å, and the residual (black continuous line, with values close to zero) over the range of the fit.

Table S1 Structural parameters (interatomic distance, r_{jk}, coordination number, n_{jk}, and RMS variation in distance, $\left\langle u_{jk}^2 \right\rangle^{½}$) for the fit to the experimental differential correlation function, $D_{exp}(r)$, of Al_2O_3 over the distance range from 0.50 to 2.25 Å. The Al-O interatomic distances for the average structure, according to a literature report of the crystal structure (Thompson *et al.*, 1987), are given, together with the refined distances from the fit. (Statistical errors from the fits are given in brackets.)

Atom pair *j*-*k*	r_{jk} / Å		n_{jk}	$\left\langle u_{jk}^2 \right\rangle^{½}$ / Å	Structural description
	Average structure	Fit			
$(Al\text{-}O)_1$	1.852	1.8550(9)	3	0.061(1)	Short bond in AlO_6 octahedron
$(Al\text{-}O)_2$	1.973	1.969(1)	3	0.076(2)	Long bond in AlO_6 octahedron

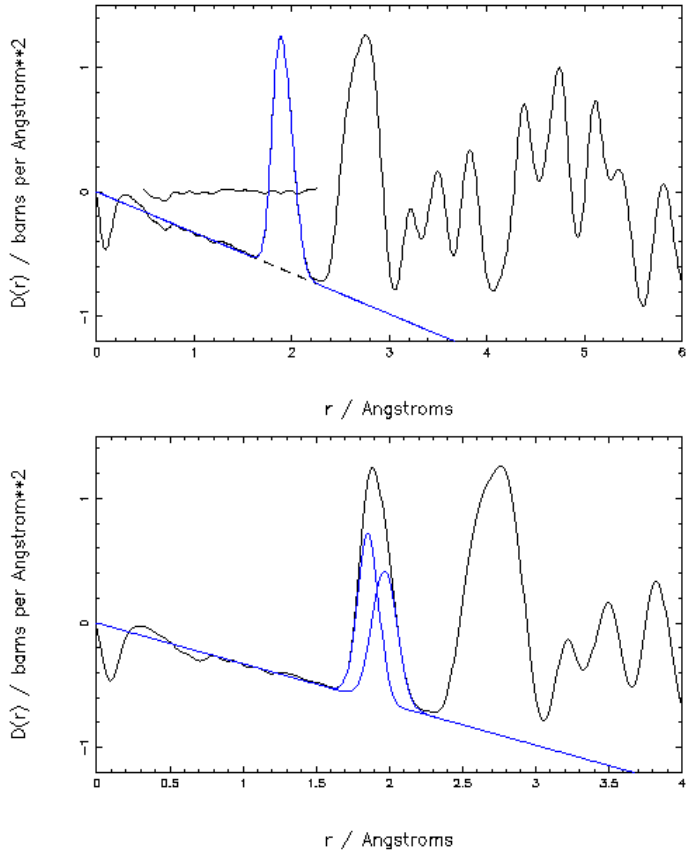

Figure S3 The experimental differential correlation function, $D_{exp}(r)$, for Al_2O_3 (black continuous line). a) Also shown is the total function (blue) fitted over the distance range 0.50 Å to 2.25 Å, the fitted average density term (black dashed line), and the residual (black continuous line, with values close to zero) over the range of the fit. b) Also shown are the individual component peaks of the fit (blue).

Table S2 Structural parameters (interatomic distance, r_{jk}, coordination number, n_{jk}, and RMS variation in distance, $\left\langle u_{jk}^2 \right\rangle^{½}$) for the fit to the experimental differential correlation function, $D_{exp}(r)$, of Al_2O_3 over the distance range from 0.50 to 2.89 Å. A dashed horizontal line is used to separate the distances for the different peak manifolds in the correlation function. The interatomic distances for the average structure, according to a literature report of the crystal structure (Thompson *et al.*, 1987), are given, and only the Al-O distances were refined in the fit. (Statistical errors from the fits are given in brackets.)

Atom pair *j-k*	r_{jk} / Å		n_{jk}	$\left\langle u_{jk}^2 \right\rangle^{½}$ / Å	Structural description
	Average structure	Fit			
$(Al\text{-}O)_1$	1.852	1.8550(9)	3	0.061(1)	Short bond in AlO_6 octahedron
$(Al\text{-}O)_2$	1.973	1.969(1)	3	0.076(1)	Long bond in AlO_6 octahedron
$(O\text{-}O)_1$	2.540		2	0.077(2)	Edges of face shared between two octahedra
$(O\text{-}O)_2$	2.623		2	0.094(2)	Edge shared between two octahedra
$(Al\text{-}Al)_1$	2.645		1	0.11(3)[a]	Distance across shared face
$(O\text{-}O)_3$	2.722		4	0.088(4)	Octahedron edge, not shared with another octahedron
$(Al\text{-}Al)_2$	2.789		3	0.11(3)[a]	Distance across shared edge
$(O\text{-}O)_4$	2.857		4	0.079(3)	Octahedron edge, not shared with another octahedron

[a]Values constrained to be equal.

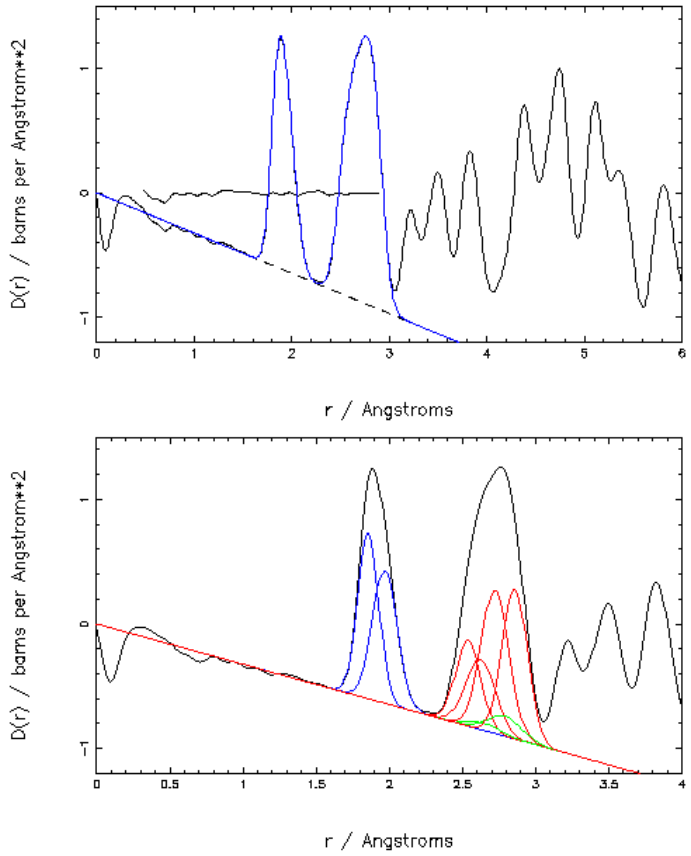

Figure S4 The experimental differential correlation function, $D_{exp}(r)$, for Al_2O_3 (black continuous line). a) Also shown is the total function (blue) fitted over the distance range 0.50 Å to 2.89 Å, the fitted average density term (black dashed line), and the residual (black continuous line, with values close to zero) over the range of the fit. b) Also shown are the individual component peaks of the fit, using the same colour key for pairs of elements as in Fig. 2b.

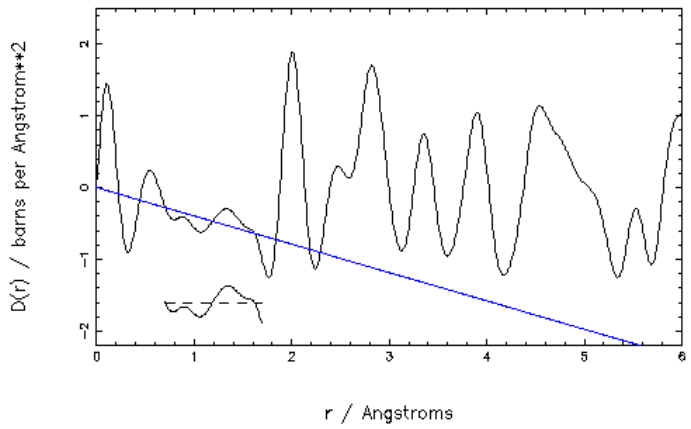

Figure S5 The experimental differential correlation function, $D_{exp}(r)$, for isotopically enriched Sr_2IrO_4 (black continuous line). a) Also shown is the fit (blue) to the experimental data over the distance range 0.70 Å to 1.70 Å, and the residual (black continuous line, displaced vertically by –1.6 units for visibility, with the zero level shown as a horizontal black short dashed line) over the range of the fit.

Table S3 Structural parameters (interatomic distance, r_{jk}, coordination number, n_{jk}, and RMS variation in distance, $\left\langle u_{jk}^2 \right\rangle^{½}$) for the fit to the experimental differential correlation function, $D_{exp}(r)$, for isotopically enriched Sr_2IrO_4 over the distance range 0.70 to 2.19 Å. The interatomic distances and coordination numbers, obtained by Rietveld refinement (Table 3), are given, and were not refined in the fit. (Statistical errors from the fits are given in brackets.)

Atom pair *j*-*k*	r_{jk} / Å	n_{jk}	$\left\langle u_{jk}^2 \right\rangle^{½}$ / Å	Structural description
Ir-O	2.005[a]	6	0.070(3)	Average Ir-O distance in IrO_6 octahedron

[a]Value is an appropriately weighted average for equatorial and axial Ir-O bonds

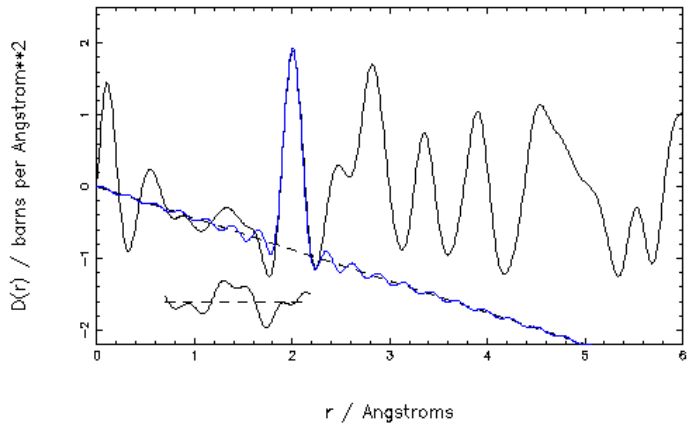

Figure S6 The experimental differential correlation function, $D_{exp}(r)$, for isotopically enriched Sr_2IrO_4 (black continuous line). a) Also shown is the fit (blue) to the experimental data over the distance range 0.70 Å to 2.19 Å, the fitted average density term (black long dashed line), and the residual (black continuous line, displaced vertically by –1.6 units for visibility, with the zero level shown as a horizontal black short dashed line) over the range of the fit.

Table S4 Structural parameters (interatomic distance, r_{jk}, coordination number, n_{jk}, and RMS variation in distance, $\left\langle u_{jk}^2 \right\rangle^{½}$) for the fit to the experimental differential correlation function, $D_{exp}(r)$, for isotopically enriched Sr_2IrO_4 over the distance range 0.70 to 3.10 Å. A dashed horizontal line is used to separate the distances for the different peak manifolds in the correlation function. The interatomic distances and coordination numbers, obtained by Rietveld refinement (Table 3), are given, and were not refined in the fit. (Statistical errors from the fits are given in brackets.)

Atom pair *j-k*	r_{jk} / Å	n_{jk}	$\left\langle u_{jk}^2 \right\rangle^{½}$ / Å	Structural description
Ir-O	2.005[a]	6	0.069(2)	Average Ir-O distance in IrO_6 octahedron
$(Sr\text{-}O)_1$	2.475[b]	3	0.083(3)	Shortest bond in irregular SrO_9 polyhedron
$(Sr\text{-}O)_2$	2.752	4	0.108(4)	Intermediate bond in irregular SrO_9 polyhedron
$(O\text{-}O)_1$	2.798	2	0.097(4)[c]	O2-O2 distance between any pair of equatorial oxygens in IrO_6 octahedron
$(O\text{-}O)_2$	2.857	4	0.097(4)[c]	O1-O2 distance from axial oxygen to equatorial oxygen in IrO_6 octahedron
$(Sr\text{-}O)_3$	3.009	2	0.083(8)	Longest bond in irregular SrO_9 polyhedron

[a]Value is an appropriately weighted average for equatorial and axial Ir-O bonds

[b]Value is an appropriate average of two closely similar Sr-O bond lengths

[c]Values constrained to be equal.

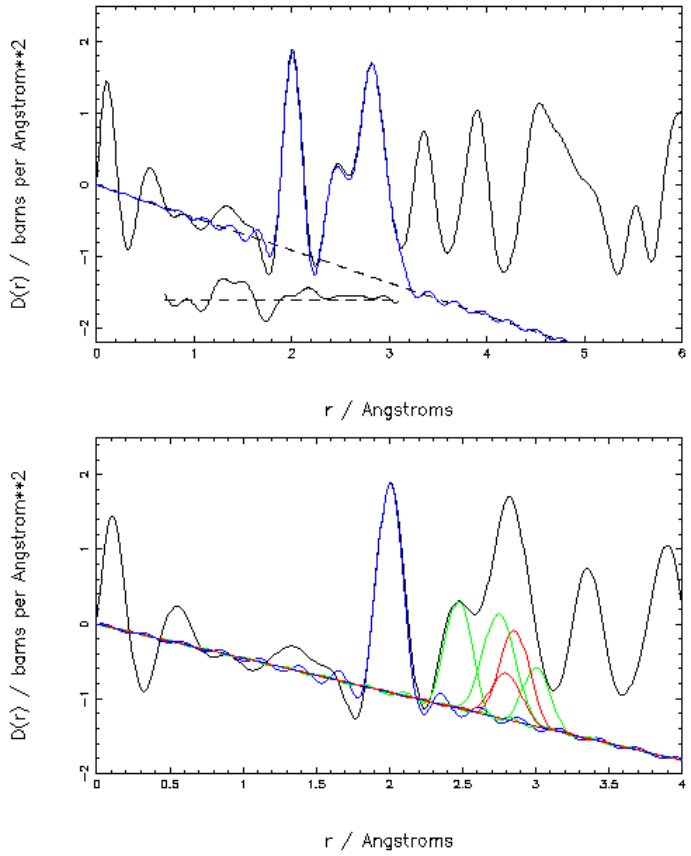

Figure S7 The experimental differential correlation function, $D_{exp}(r)$, for isotopically enriched Sr_2IrO_4 (black continuous line). a) Also shown is the total function (blue) fitted over the distance range 0.70 Å to 3.10 Å, the fitted average density term (sloping black long dashed line), and the residual (black continuous line, displaced vertically by –1.6 units for visibility, with the zero level shown as a horizontal black short dashed line) over the range of the fit. b) Also shown are the individual component peaks of the fit, using the same colour key for pairs of elements as in Fig. 3b.

References

Hannon, A. C. (2005). *Nucl. Instrum. Meth. A* **551**, 88-107.
Swanson, H. E., Fuyat, R. K. & Ugrinic, G. M. (1955). *National Bureau of Standards (U.S.), Circular* **539-IV**, 9-10.
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