IUCrData

ISSN 2414-3146

Refinement of the crystal structure of UOs_2 from single-crystal X-ray diffraction data

Sergei I. Ivlev,[a] Matthias Conrad,[a] Carsten Wolf[b] and Florian Kraus[c]*

[a]Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany, [b]Bruker AXS SE, Östliche Rheinbrückenstrasse 49, 76187 Karlsruhe, Germany, and [c]Anorganische Chemie, Fluorchemie, Institut für Anorganische Chemie, Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany. *Correspondence e-mail: fkraus@uni-bonn.de

Received 9 June 2026
Accepted 2 July 2026

Edited by M. Weil, Vienna University of Technology, Austria

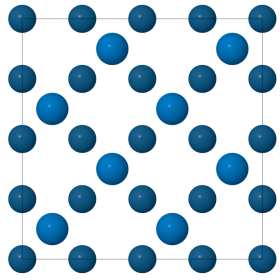
Keywords: crystal structure; intermetallics; single-crystal X-ray diffraction; redetermination; $MgCu_2$ structure type.

CCDC reference: 2567529

Structural data: full structural data are available from iucrdata.iucr.org

Single crystals of uranium diosmium, UOs_2, were obtained during an investigation of the uranium-osmium binary system by an interaction of uranium metal with osmium metal in an arc furnace and subsequent annealing. The refinement of the crystal structure of UO_2 was carried out for the first time using single-crystal X-ray diffraction data. In contrast to previous structure reports based on powder diffraction data, the U and Os atoms were refined with all U^{ij} terms of the displacement parameters considered. UOs_2 adopts the $MgCu_2$ structure type.

3D view



Structure description

According to the Inorganic Crystal Structure Database (ICSD; Zagorac *et al.*, 2019), the first crystal structure determination of the binary phase UOs_2 was carried out by Heal & Williams (1955) using a powder sample and a diffractometer operated with Co radiation. They reported the compound to crystallize in the space group $Fd\overline{3}m$ (No. 227) with a = 7.5125 (5) Å, V = 423.99 Å^3, Z = 8 at 297 K belonging to the $MgCu_2$ structure type. Subsequent structure reports confirmed this finding with the unit-cell parameter to be in very close agreement with the one originally reported: 7.514 Å [Knapton, 1963; room-temperature data, no standard uncertainty (s.u.) given]; 7.501 (4) Å (Holleck *et al.*, 1975; room-temperature data); 7.514 Å (Mentink *et al.*, 1992; room-temperature data, no s.u. given); 7.4919 (Nishioka *et al.*, 1994; room-temperature data, no s.u. given). Nishioka *et al.* (1994) also reported the existence of a polymorph of UOs_2 belonging to the $MgZn_2$ structure type [space group $P6_3/mmc$ (No. 194) with a = 5.49, c = 8.71 Å, V = 227.35 Å^3, Z = 4; room temperature data, no s.u. given]. All mentioned crystal-structure refinements were carried out on the basis of powder diffraction techniques with both Os and U atoms being refined isotropically. Although an anisotropic refinement of the U atom is

equivalent to the isotropic one due to symmetry constraints, the site symmetry of the Os atom does allow non-zero off-diagonal U^{ij} terms, when refined anisotropically. Here we report our results on the crystal-structure determination of UOs_2 using single-crystal X-ray diffraction data at 100 K that allowed to use the anisotropic approximation for the displacement parameters (Fig. 1).

The unit-cell parameter of UOs_2 obtained from the single-crystal diffraction experiment (Table 1) is in good agreement with all previously reported data. The U atom resides on the special 8*a* ($\bar{4}3m$) Wyckoff position. The Os atom occupies the special 16*d* ($.\bar{3}m$) Wyckoff position. The closest interatomic distances are U···U 3.24669 (8), Os···Os 2.65091 (7), and U···Os 3.10847 (8) Å.

Since UOs_2 is isotypic to the well known Laves phase $MgCu_2$, its crystal structure will only be described very briefly. The U atoms are arranged like the atoms in the cubic diamond structure type. The Os atoms form Os_4 tetrahedra. Their virtual centres of gravity are also arranged according to the cubic diamond structure type, and the two networks interpenetrate. Overall, the coordination number of the Os atom is 12 within a slightly distorted icosahedral coordination environment. Each Os atom resides within the centre of a U_6 ring adopting a chair conformation and is additionally surrounded by six Os atoms in the shape of a trigonal antiprism. Overall, the coordination number of the U atom is 16. Each U atom is surrounded tetrahedrally by four U atoms and by twelve Os atoms in the shape of a fourfold truncated tetrahedron, which is sometimes referred to as the Friauf polyhedron (Wells, 1975).

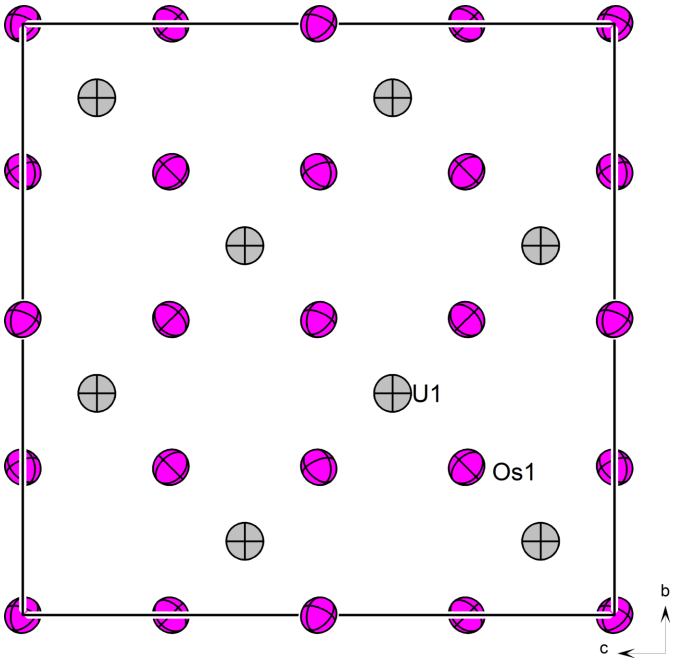


Figure 1
Crystal structure of UOs_2 in a projection along [100]. Displacement ellipsoids are shown at the 90% probability level.

Table 1
Experimental details.

Crystal data	
Chemical formula	UOs_2
M_r	618.43
Crystal system, space group	Cubic, $Fd\bar{3}m$
Temperature (K)	100
a (Å)	7.4979 (2)
V (Å^3)	421.52 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	196.43
Crystal size (mm)	0.05 × 0.04 × 0.03
Data collection	
Diffractometer	Bruker D8 VENTURE
Absorption correction	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.014, 0.127
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2221, 69, 66
R_{int}	0.083
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.830
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.047, 1.40
No. of reflections	69
No. of parameters	5
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.92, −2.16

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2019), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 2022) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

Single crystals of UOs_2 were obtained by a direct reaction between stoichiometric amounts of uranium and osmium metal powders in an arc furnace. The polycrystalline reaction product was subsequently annealed in a tantalum ampule at 1073 K for 11 d and crushed in oil under a microscope to select a single crystal suitable for the diffraction study.

Refinement

Details of data collection and structure refinement are given in Table 1.

Acknowledgements

We thank the DFG for very generous funding over the years.

Funding information

Funding for this research was provided by: Deutsche Forschungsgemeinschaft.

References

Brandenburg, K. (2022). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2019). *SAINT*. Bruker AXS, Karlsruhe, Germany.
Bruker (2023). *APEX5*. Bruker AXS, Karlsruhe, Germany.
Heal, T. J. & Williams, G. I. (1955). *Acta Cryst.* **8**, 494–498.

Holleck, H., Kleykamp, H. & Franco, J. I. (1975). *Z. Metallkd.* **66**, 298–302.
Knapton, A. G. (1963). *J. Nucl. Mater.* **9**, 309–319.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Mentink, S. A. M., Nieuwenhuys, G. J. & Mydosh, J. A. (1992). *J. Magn. Magn. Mater.* **104–107**, 697–698.
Nishioka, T., Kimura, K., Matsui, H. & Kontani, M. (1994). *J. Phys. Soc. Jpn* **63**, 2722–2730.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Wells, A. F. (1975). *Structural Inorganic Chemistry*, 4th ed., pp. 1034–1038 Oxford: Clarendon Press.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Zagorac, D., Müller, H., Ruehl, S., Zagorac, J. & Rehme, S. (2019). *J. Appl. Cryst.* **52**, 918–925.

full crystallographic data

IUCrData (2026). **11**, x260691 [https://doi.org/10.1107/S2414314626006917]

Refinement of the crystal structure of UOs_2 from single-crystal X-ray diffraction data

Sergei I. Ivlev, Matthias Conrad, Carsten Wolf and Florian Kraus

Uranium diosmium

Crystal data

UOs_2
M_r = 618.43
Cubic, $Fd\bar{3}m$
a = 7.4979 (2) Å
V = 421.52 (3) Å^3
Z = 8
$F(000)$ = 1952
D_x = 19.490 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2037 reflections
θ = 4.7–36.2°
μ = 196.43 mm^{-1}
T = 100 K
Block, metallic grey
0.05 × 0.04 × 0.03 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: microfocus X-ray tube
ω and φ scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.014, T_{max} = 0.127
2221 measured reflections
69 independent reflections
66 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 36.2°, θ_{min} = 4.7°
h = −11→10
k = −10→11
l = −12→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.047
S = 1.40
69 reflections
5 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0161P)^2 + 10.8153P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.92 e Å^{-3}
$\Delta\rho_{min}$ = −2.16 e Å^{-3}
Extinction correction: SHELXL2019/2 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00055 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
U1	0.875000	0.375000	0.375000	0.0088 (3)
Os1	0.500000	0.250000	0.250000	0.0082 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.0088 (3)	0.0088 (3)	0.0088 (3)	0.000	0.000	0.000
Os1	0.0082 (3)	0.0082 (3)	0.0082 (3)	0.00062 (12)	0.00062 (12)	−0.00062 (12)

Geometric parameters (Å, º)

U1—Os1^{i}	3.1085 (1)	U1—Os1^{xi}	3.1085 (1)
U1—Os1	3.1085 (1)	U1—U1^{xii}	3.2467 (1)
U1—Os1^{ii}	3.1085 (1)	U1—U1^{xiii}	3.2467 (1)
U1—Os1^{iii}	3.1085 (1)	U1—U1^{xiv}	3.2467 (1)
U1—Os1^{iv}	3.1085 (1)	U1—U1^{xv}	3.2467 (1)
U1—Os1^{v}	3.1085 (1)	Os1—Os1^{xvi}	2.6509 (1)
U1—Os1^{vi}	3.1085 (1)	Os1—Os1^{ix}	2.6509 (1)
U1—Os1^{vii}	3.1085 (1)	Os1—Os1^{xvii}	2.6509 (1)
U1—Os1^{viii}	3.1085 (1)	Os1—Os1^{i}	2.6509 (1)
U1—Os1^{ix}	3.1085 (1)	Os1—Os1^{ii}	2.6509 (1)
U1—Os1^{x}	3.1085 (1)	Os1—Os1^{xviii}	2.6509 (1)
Os1^{i}—U1—Os1	50.5	Os1^{ii}—U1—U1^{xiv}	58.5
Os1^{i}—U1—Os1^{ii}	50.5	Os1^{iii}—U1—U1^{xiv}	150.5
Os1—U1—Os1^{ii}	50.5	Os1^{iv}—U1—U1^{xiv}	58.518 (1)
Os1^{i}—U1—Os1^{iii}	144.9	Os1^{v}—U1—U1^{xiv}	100.025 (1)
Os1—U1—Os1^{iii}	95.2	Os1^{vi}—U1—U1^{xiv}	100.025 (1)
Os1^{ii}—U1—Os1^{iii}	117.0	Os1^{vii}—U1—U1^{xiv}	58.518 (1)
Os1^{i}—U1—Os1^{iv}	95.2	Os1^{viii}—U1—U1^{xiv}	150.5
Os1—U1—Os1^{iv}	144.9	Os1^{ix}—U1—U1^{xiv}	150.5
Os1^{ii}—U1—Os1^{iv}	117.0	Os1^{x}—U1—U1^{xiv}	58.5
Os1^{iii}—U1—Os1^{iv}	117.0	Os1^{xi}—U1—U1^{xiv}	58.5
Os1^{i}—U1—Os1^{v}	95.2	U1^{xii}—U1—U1^{xiv}	109.471 (1)
Os1—U1—Os1^{v}	117.0	U1^{xiii}—U1—U1^{xiv}	109.5
Os1^{ii}—U1—Os1^{v}	144.9	Os1^{i}—U1—U1^{xv}	58.5
Os1^{iii}—U1—Os1^{v}	95.2	Os1—U1—U1^{xv}	58.5
Os1^{iv}—U1—Os1^{v}	50.5	Os1^{ii}—U1—U1^{xv}	100.0
Os1^{i}—U1—Os1^{vi}	144.9	Os1^{iii}—U1—U1^{xv}	100.0
Os1—U1—Os1^{vi}	117.0	Os1^{iv}—U1—U1^{xv}	100.025 (1)
Os1^{ii}—U1—Os1^{vi}	95.2	Os1^{v}—U1—U1^{xv}	58.5
Os1^{iii}—U1—Os1^{vi}	50.5	Os1^{vi}—U1—U1^{xv}	150.5
Os1^{iv}—U1—Os1^{vi}	95.2	Os1^{vii}—U1—U1^{xv}	150.5
Os1^{v}—U1—Os1^{vi}	117.0	Os1^{viii}—U1—U1^{xv}	58.5
Os1^{i}—U1—Os1^{vii}	117.0	Os1^{ix}—U1—U1^{xv}	58.5

Os1—U1—Os1^{vii}	144.9
Os1^{ii}—U1—Os1^{vii}	95.2
Os1^{iii}—U1—Os1^{vii}	95.2
Os1^{iv}—U1—Os1^{vii}	50.5
Os1^{v}—U1—Os1^{vii}	95.2
Os1^{vi}—U1—Os1^{vii}	50.5
Os1^{i}—U1—Os1^{viii}	117.0
Os1—U1—Os1^{viii}	95.2
Os1^{ii}—U1—Os1^{viii}	144.9
Os1^{iii}—U1—Os1^{viii}	50.5
Os1^{iv}—U1—Os1^{viii}	95.2
Os1^{v}—U1—Os1^{viii}	50.5
Os1^{vi}—U1—Os1^{viii}	95.2
Os1^{vii}—U1—Os1^{viii}	117.0
Os1^{i}—U1—Os1^{ix}	95.2
Os1—U1—Os1^{ix}	50.5
Os1^{ii}—U1—Os1^{ix}	95.2
Os1^{iii}—U1—Os1^{ix}	50.5
Os1^{iv}—U1—Os1^{ix}	144.9
Os1^{v}—U1—Os1^{ix}	95.2
Os1^{vi}—U1—Os1^{ix}	95.2
Os1^{vii}—U1—Os1^{ix}	144.9
Os1^{viii}—U1—Os1^{ix}	50.5
Os1^{i}—U1—Os1^{x}	95.216 (1)
Os1—U1—Os1^{x}	95.2
Os1^{ii}—U1—Os1^{x}	50.5
Os1^{iii}—U1—Os1^{x}	95.2
Os1^{iv}—U1—Os1^{x}	95.2
Os1^{v}—U1—Os1^{x}	144.9
Os1^{vi}—U1—Os1^{x}	50.5
Os1^{vii}—U1—Os1^{x}	50.5
Os1^{viii}—U1—Os1^{x}	144.9
Os1^{ix}—U1—Os1^{x}	117.0
Os1^{i}—U1—Os1^{xi}	50.5
Os1—U1—Os1^{xi}	95.2
Os1^{ii}—U1—Os1^{xi}	95.216 (1)
Os1^{iii}—U1—Os1^{xi}	144.9
Os1^{iv}—U1—Os1^{xi}	50.5
Os1^{v}—U1—Os1^{xi}	50.5
Os1^{vi}—U1—Os1^{xi}	144.9
Os1^{vii}—U1—Os1^{xi}	95.2
Os1^{viii}—U1—Os1^{xi}	95.2
Os1^{ix}—U1—Os1^{xi}	117.0
Os1^{x}—U1—Os1^{xi}	117.0
Os1^{i}—U1—U1^{xii}	150.5
Os1—U1—U1^{xii}	150.5
Os1^{ii}—U1—U1^{xii}	150.5
Os1^{iii}—U1—U1^{xii}	58.5
Os1^{x}—U1—U1^{xv}	150.5
Os1^{xi}—U1—U1^{xv}	58.5
U1^{xii}—U1—U1^{xv}	109.471 (1)
U1^{xiii}—U1—U1^{xv}	109.5
U1^{xiv}—U1—U1^{xv}	109.5
Os1^{xvi}—Os1—Os1^{ix}	180.0
Os1^{xvi}—Os1—Os1^{xvii}	120.0
Os1^{ix}—Os1—Os1^{xvii}	60.0
Os1^{xvi}—Os1—Os1^{i}	60.0
Os1^{ix}—Os1—Os1^{i}	120.0
Os1^{xvii}—Os1—Os1^{i}	180.0
Os1^{xvi}—Os1—Os1^{ii}	60.0
Os1^{ix}—Os1—Os1^{ii}	120.0
Os1^{xvii}—Os1—Os1^{ii}	120.0
Os1^{i}—Os1—Os1^{ii}	60.0
Os1^{xvi}—Os1—Os1^{xviii}	120.0
Os1^{ix}—Os1—Os1^{xviii}	60.0
Os1^{xvii}—Os1—Os1^{xviii}	60.0
Os1^{i}—Os1—Os1^{xviii}	120.0
Os1^{ii}—Os1—Os1^{xviii}	180.0
Os1^{xvi}—Os1—U1	115.2
Os1^{ix}—Os1—U1	64.8
Os1^{xvii}—Os1—U1	115.2
Os1^{i}—Os1—U1	64.8
Os1^{ii}—Os1—U1	64.8
Os1^{xviii}—Os1—U1	115.2
Os1^{xvi}—Os1—U1^{xix}	64.8
Os1^{ix}—Os1—U1^{xix}	115.2
Os1^{xvii}—Os1—U1^{xix}	64.8
Os1^{i}—Os1—U1^{xix}	115.2
Os1^{ii}—Os1—U1^{xix}	115.2
Os1^{xviii}—Os1—U1^{xix}	64.8
U1—Os1—U1^{xix}	180.0
Os1^{xvi}—Os1—U1^{xv}	115.2
Os1^{ix}—Os1—U1^{xv}	64.8
Os1^{xvii}—Os1—U1^{xv}	115.2
Os1^{i}—Os1—U1^{xv}	64.8
Os1^{ii}—Os1—U1^{xv}	115.2
Os1^{xviii}—Os1—U1^{xv}	64.8
U1—Os1—U1^{xv}	63.0
U1^{xix}—Os1—U1^{xv}	117.0
Os1^{xvi}—Os1—U1^{xx}	64.8
Os1^{ix}—Os1—U1^{xx}	115.239 (1)
Os1^{xvii}—Os1—U1^{xx}	64.8
Os1^{i}—Os1—U1^{xx}	115.2
Os1^{ii}—Os1—U1^{xx}	64.8
Os1^{xviii}—Os1—U1^{xx}	115.2
U1—Os1—U1^{xx}	117.0

Os1^{iv}—U1—U1^{xii}	58.5	U1^{xix}—Os1—U1^{xx}	63.0
Os1^{v}—U1—U1^{xii}	58.5	U1^{xv}—Os1—U1^{xx}	180.0
Os1^{vi}—U1—U1^{xii}	58.5	Os1^{xvi}—Os1—U1^{xxi}	64.8
Os1^{vii}—U1—U1^{xii}	58.5	Os1^{ix}—Os1—U1^{xxi}	115.2
Os1^{viii}—U1—U1^{xii}	58.5	Os1^{xvii}—Os1—U1^{xxi}	115.2
Os1^{ix}—U1—U1^{xii}	100.025 (1)	Os1^{i}—Os1—U1^{xxi}	64.8
Os1^{x}—U1—U1^{xii}	100.0	Os1^{ii}—Os1—U1^{xxi}	115.2
Os1^{xi}—U1—U1^{xii}	100.0	Os1^{xviii}—Os1—U1^{xxi}	64.8
Os1^{i}—U1—U1^{xiii}	100.0	U1—Os1—U1^{xxi}	117.0
Os1—U1—U1^{xiii}	58.518 (1)	U1^{xix}—Os1—U1^{xxi}	63.0
Os1^{ii}—U1—U1^{xiii}	58.518 (1)	U1^{xv}—Os1—U1^{xxi}	63.0
Os1^{iii}—U1—U1^{xiii}	58.5	U1^{xx}—Os1—U1^{xxi}	117.0
Os1^{iv}—U1—U1^{xiii}	150.5	Os1^{xvi}—Os1—U1^{xiii}	115.2
Os1^{v}—U1—U1^{xiii}	150.5	Os1^{ix}—Os1—U1^{xiii}	64.8
Os1^{vi}—U1—U1^{xiii}	58.5	Os1^{xvii}—Os1—U1^{xiii}	64.8
Os1^{vii}—U1—U1^{xiii}	100.0	Os1^{i}—Os1—U1^{xiii}	115.2
Os1^{viii}—U1—U1^{xiii}	100.0	Os1^{ii}—Os1—U1^{xiii}	64.8
Os1^{ix}—U1—U1^{xiii}	58.5	Os1^{xviii}—Os1—U1^{xiii}	115.2
Os1^{x}—U1—U1^{xiii}	58.5	U1—Os1—U1^{xiii}	63.0
Os1^{xi}—U1—U1^{xiii}	150.5	U1^{xix}—Os1—U1^{xiii}	117.0
U1^{xii}—U1—U1^{xiii}	109.471 (1)	U1^{xv}—Os1—U1^{xiii}	117.0
Os1^{i}—U1—U1^{xiv}	58.5	U1^{xx}—Os1—U1^{xiii}	63.0
Os1—U1—U1^{xiv}	100.0	U1^{xxi}—Os1—U1^{xiii}	180.0

Symmetry codes: (i) −*x*+5/4, *y*, −*z*+1/4; (ii) −*x*+5/4, −*y*+1/4, *z*; (iii) −*x*+5/4, −*y*+3/4, *z*+1/2; (iv) −*x*+7/4, −*y*+3/4, *z*; (v) *x*+1/2, *y*+1/2, *z*; (vi) *x*+1/2, *y*, *z*+1/2; (vii) −*x*+7/4, *y*, −*z*+3/4; (viii) −*x*+5/4, *y*+1/2, −*z*+3/4; (ix) *x*, −*y*+3/4, −*z*+3/4; (x) *x*+1/2, −*y*+1/4, −*z*+3/4; (xi) *x*+1/2, −*y*+3/4, −*z*+1/4; (xii) −*x*+2, −*y*+1, −*z*+1; (xiii) −*y*+1, *x*−3/4, *z*+1/4; (xiv) −*x*+2, −*y*+1/2, −*z*+1/2; (xv) −*x*+3/2, −*y*+1, −*z*+1/2; (xvi) *x*, −*y*+1/4, −*z*+1/4; (xvii) −*x*+3/4, *y*, −*z*+3/4; (xviii) −*x*+3/4, −*y*+3/4, *z*; (xix) −*x*+1, −*y*+1/2, −*z*+1/2; (xx) *x*−1/2, *y*−1/2, *z*; (xxi) *x*−1/2, *y*, *z*−1/2.