Towards inert and preorganized *d*-block-containing receptors for trivalent lanthanides: The synthesis and characterisation of triple-helical monometallic Os^{II} and bimetallic Os^{II}-Ln^{III} complexes

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Supporting information

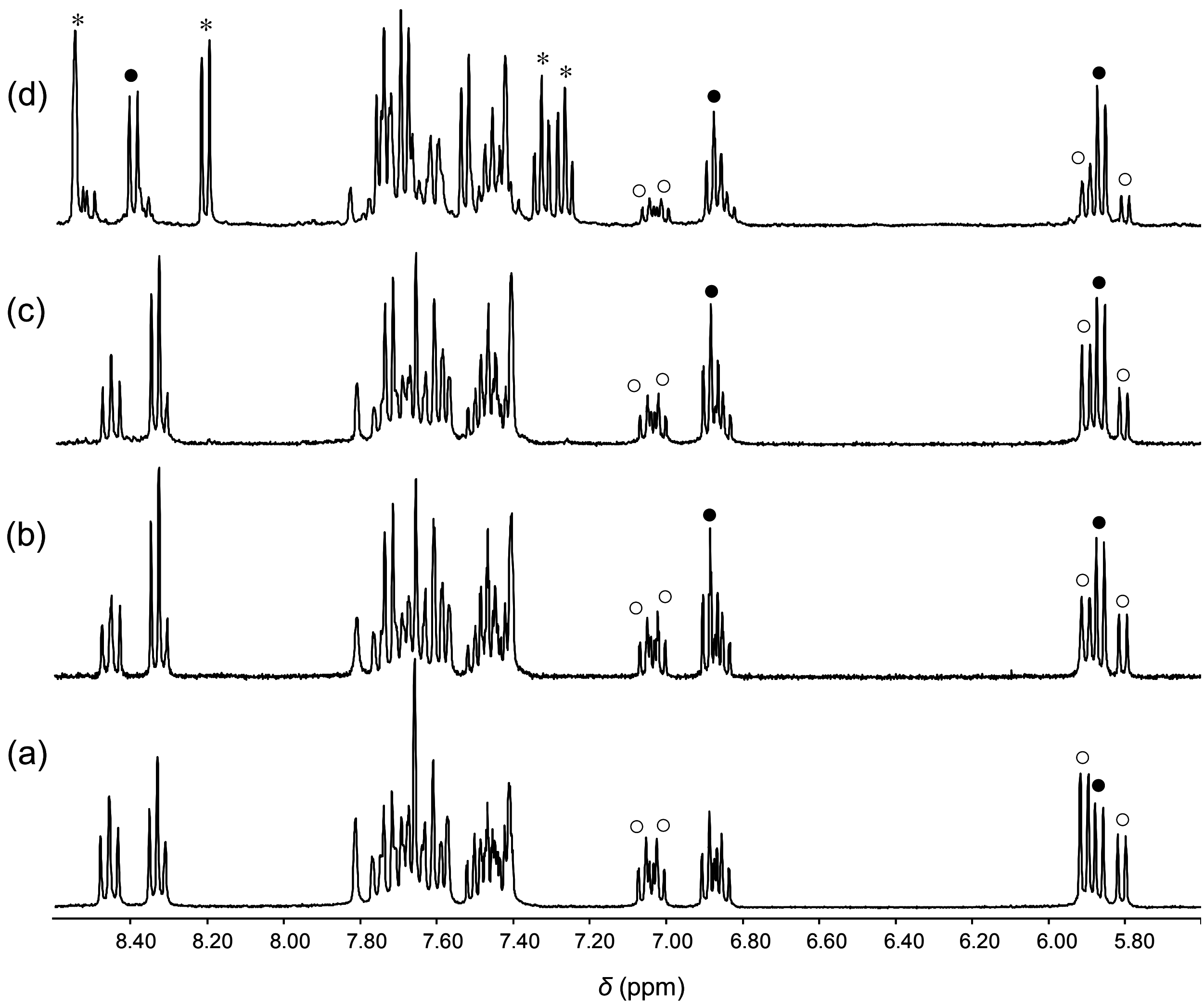


Figure S1. [1]H NMR spectra of crude mixtures obtained after reaction of *trans*-[$Os^{II}Cl_2(DMSO)_4$] with **L1** in (a) ethylene glycol (180 °C, 1 bar, 16 hrs, complex as PF_6^- salt), (b) propan-1,3-diol (180 °C, 1 bar, 16 hrs, complex as PF_6^- salt), (c) butan-1,4-diol (180 °C, 1 bar, 16 hrs, complex as PF_6^- salt) and (d) ethanol (180 °C, 17-20 bar, 16 hrs, complex as Cl^- salt) showing relative proportions of *mer*-[Os(**L1**)$_3$]$^{2+}$ (○), *fac*-[Os(**L1**)$_3$]$^{2+}$ (●) and free ligand (*).

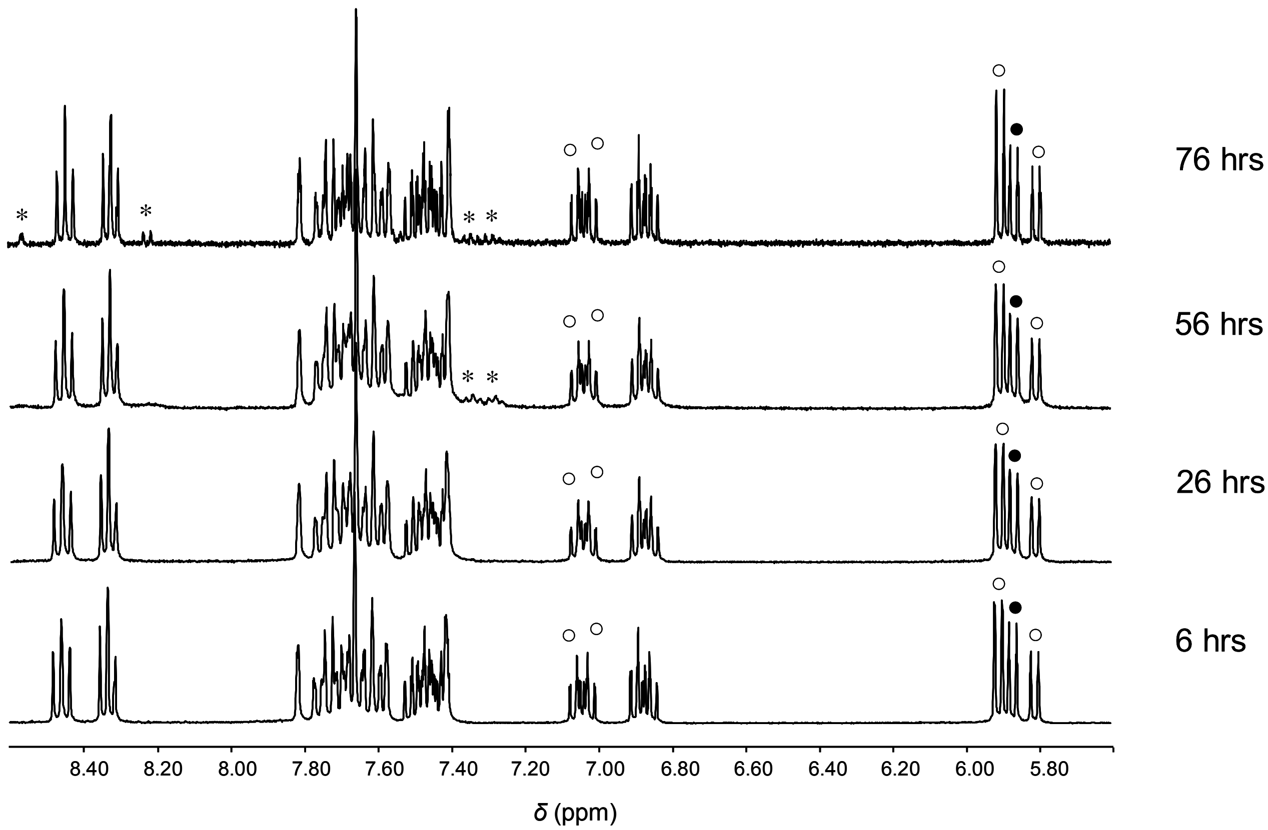


Figure S2. ^{1}H NMR spectra showing variation in ratio of *mer-/fac-* isomers as a function of time and eventual complex decomposition during reaction of (3:1) **L1** with [Os(DMSO)$_4$Cl$_2$] (ethylene glycol, 180 °C). Selected peaks due to *mer*-[Os(**L1**)$_3$]$^{2+}$ (○), *fac*-[Os(**L1**)$_3$]$^{2+}$ (●) and free ligand (∗) are marked to highlight changes.

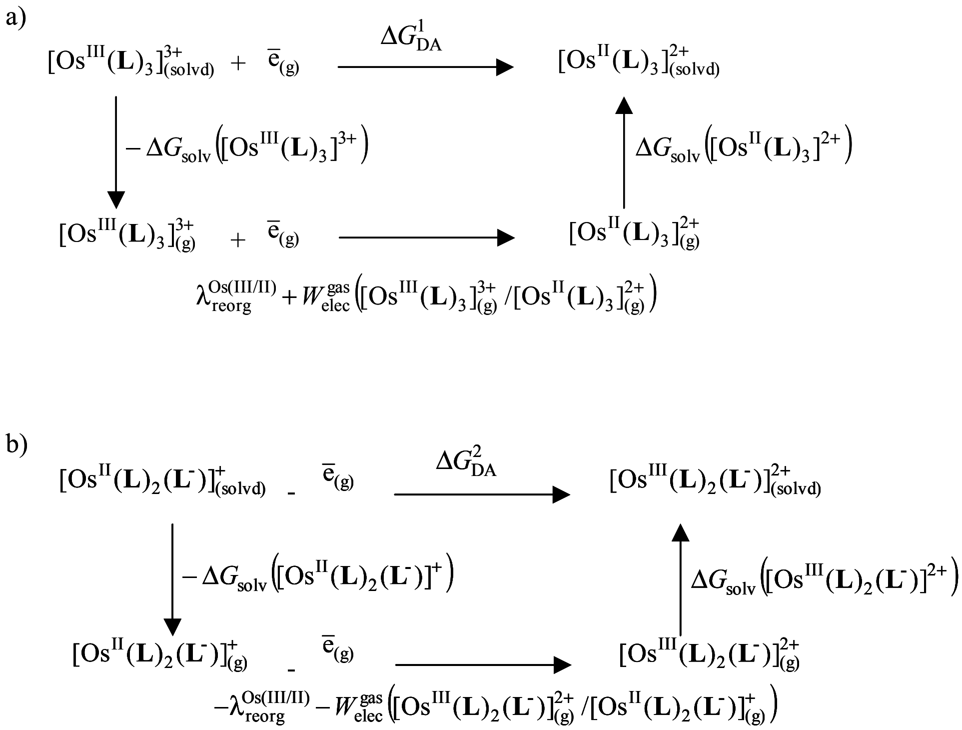


Figure S3. *Born-Haber* cycles for the estimations of a) ΔG^{1}_{DA} (eq 6) and b) ΔG^{2}_{DA} (eq 7).

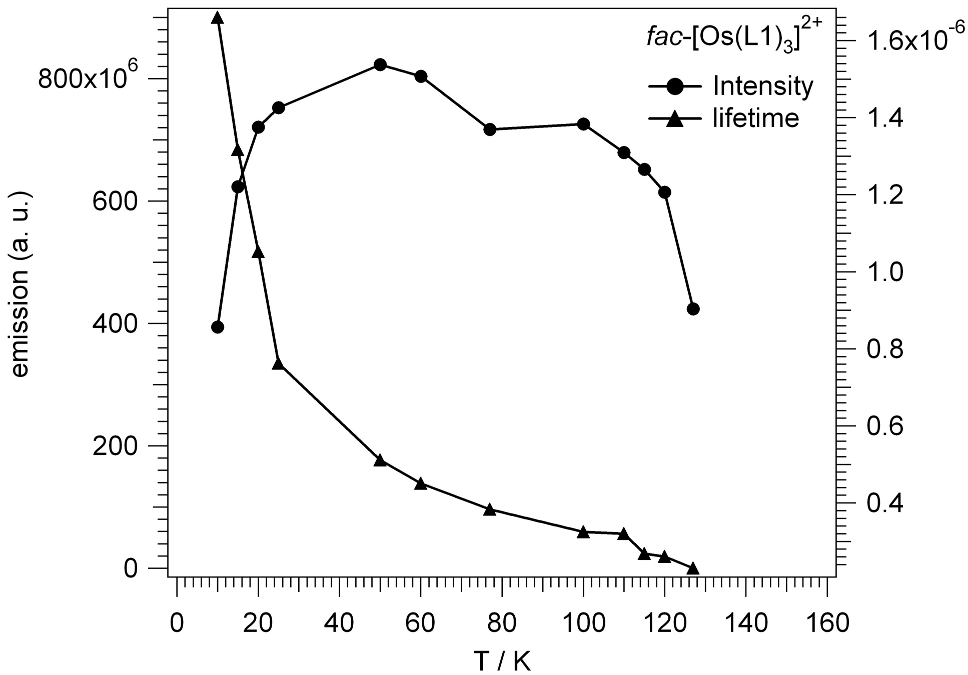


Figure S4. Plot of luminescence lifetime τ *vs* temperature for $[Os(\mathbf{L1})_3]^{2+}$.

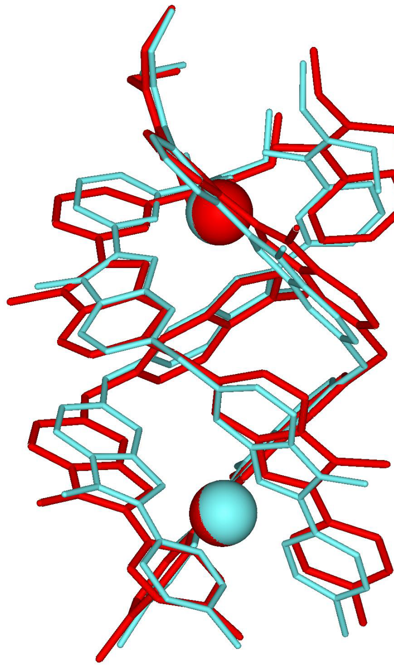


Figure S5. Optimised super-imposition of helicates *HHH*-$[OsLu(\mathbf{L2})_3]^{5+}$ (red) and *HHH*-$[RuLu(\mathbf{L2})_3]^{5+}$ (blue).

Table S1. Selected geometric parameters for *fac*-$[Os(\mathbf{L1})_3]^{2+}$ and Λ-*mer*-$[Os(\mathbf{L1})_3]^{2+}$ and $[Os(bipy)_3]^{2+}$ in parentheses.[a]

fac-$[Os(\mathbf{L1})_3]^{2+}$			
Angles ϕ (°)			
R^1-Os1-R^2 [b]	177.2 (180)		
Angles θ_i (°)			
R^1-Os1-N2a	60.0 (59.6)	R^2-Os1-N3a	58.45 (59.6)
R^1-Os1-N2b	59.2 (59.6)	R^2-Os1-N3b	57.79 (59.6)
R^1-Os1-N2c	62.3 (59.6)	R^2-Os1-N3c	59.70 (59.6)
Angles ω_{ij} (°) (intra-)			
proj[N2a]-Os1-proj[N3a][c]	50.48 (51.2)		
proj[N2b]-Os1-proj[N3b]	49.30 (51.2)		
proj[N2c]-Os1-proj[N3c]	50.71 (51.2)		
Angles ω_{ij} (°) (inter-)			
proj[N2a]-Os1-proj[N2b]	117.1		
proj[N2a]-Os1-proj[N2c]	121.7		
proj[N2b]-Os1-proj[N2c]	121.2		
proj[N3a]-Os1-proj[N3b]	118.3		
proj[N3a]-Os1-proj[N3c]	121.9		
proj[N3b]-Os1-proj[N3c]	119.8		
proj[N2a]-Os1-proj[N3b]	67.8		
proj[N2a]-Os1-proj[N3c]	172.4		
proj[N2b]-Os1-proj[N3a]	167.6		
proj[N2b]-Os1-proj[N3c]	70.5		
proj[N2c]-Os1-proj[N3a]	71.2		
proj[N2c]-Os1-proj[N3b]	170.5		

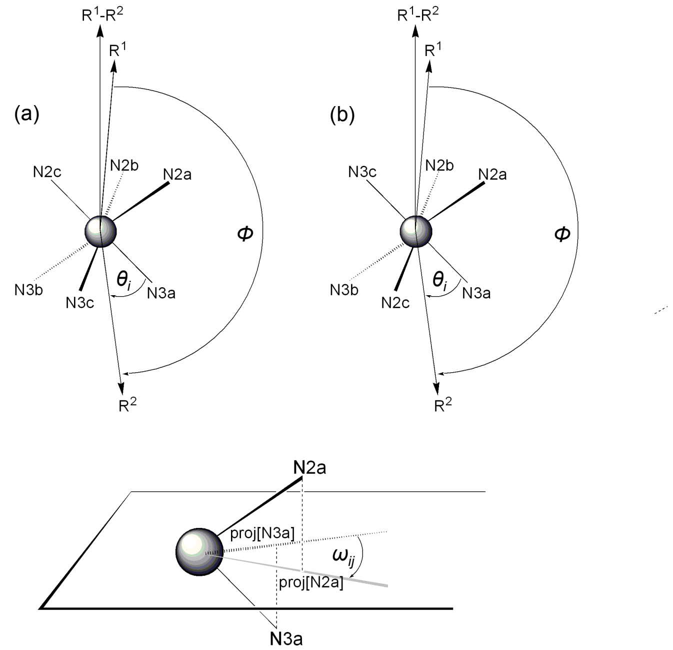
Table S1. (cont.)

Λ-*mer*-$[Os(\mathbf{L1})_3]^{2+}$			
Angles ϕ (°)			
R^1-Os1-R^2	177.9 (180)		
Angles θ_i (°)			
R^1-Os1-N2a	62.18 (59.6)	R^2-Os1-N3a	60.79 (59.6)
R^1-Os1-N2b	60.26 (59.6)	R^2-Os1-N3b	60.11 (59.6)
R^1-Os1-N3c	59.43 (59.6)	R^2-Os1-N2c	58.79 (59.6)
Angles ω_{ij} (°) (intra-)			
proj[N2a]-Os1-proj[N3a]	52.08		
proj[N2b]-Os1-proj[N3b]	51.20		
proj[N2c]-Os1-proj[N3c]	50.24		
Angles ω_{ij} (°) (inter-)			
proj[N2a]-Os1-proj[N2b]	121.00		
proj[N2a]-Os1-proj[N3c]	121.57		
proj[N2b]-Os1-proj[N3c]	117.43		
proj[N3a]-Os1-proj[N3b]	121.88		
proj[N3a]-Os1-proj[N2c]	119.73		
proj[N3b]-Os1-proj[N2c]	118.39		
proj[N2a]-Os1-proj[N3b]	69.80		
proj[N2a]-Os1-proj[N2c]	171.81		
proj[N2b]-Os1-proj[N3a]	173.07		
proj[N2b]-Os1-proj[N2c]	67.19		
proj[N3c]-Os1-proj[N3a]	69.49		
proj[N3c]-Os1-proj[N3b]	168.63		

Table S1. (cont.)

	Λ-*mer*-$[Os(\mathbf{L1})_3]^{2+}$		
Angles ϕ (°)			
R^1-Os2-R^2	178.6 (180.0)		
Angles θ_i (°)			
R^1-Os2-N2d	62.04 (59.6)	R^2-Os2-N3d	62.39 (59.6)
R^1-Os2-N2e	61.25 (59.6)	R^2-Os2-N3e	59.21 (59.6)
R^1-Os2-N3f	60.57 (59.6)	R^2-Os2-N2f	60.26 (59.6)
Angles ω_{ij} (°) (intra-)			
proj[N2d]-Os2-proj[N3d]	53.32 (51.2)		
proj[N2e]-Os2-proj[N3e]	52.76 (51.2)		
proj[N2f]-Os2-proj[N3f]	51.72 (51.2)		
Angles ω_{ij} (°) (inter-)			
proj[N2d]-Os2-proj[N2e]	121.58		
proj[N2d]-Os2-proj[N3f]	120.09		
proj[N2e]-Os2-proj[N3f]	118.33		
proj[N3d]-Os2-proj[N3e]	121.02		
proj[N3d]-Os2-proj[N2f]	121.69		
proj[N3e]-Os2-proj[N2f]	117.29		
proj[N2d]-Os2-proj[N3e]	174.34		
proj[N2d]-Os2-proj[N2f]	68.36		
proj[N2e]-Os2-proj[N3d]	68.26		
proj[N2e]-Os2-proj[N2f]	170.05		
proj[N3f]-Os2-proj[N3d]	173.41		
proj[N3f]-Os2-proj[N3e]	65.57		

[a] For definitions of ϕ, θ_i, and ω_{ij} see Scheme S1 (the error is in the range 1-2 °). [b] Vectors R^i are as defined as follows: for *fac*-$[Os(L1)_3]^{2+}$, R^1 = Os1-N2a + Os1-N2b + Os1-N2c and R^2 = Os1-N3a + Os1-N3b + Os1-N3c; for *mer*-$[Os(L1)_3]^{2+}$ (the two sets of vectors for the two crystalographically independent cations are), R^1 = Os1-N2a + Os1-N2b + Os1-N3c and R^2 = Os1-N3a + Os1-N3b + Os1-N2c; R^1 = Os2-N2d + Os2-N2e + Os2-N3f and R^2 = Os2-N3d + Os2-N3e + Os2-N2f. [c] Proj[N*i*] is the projection of N*i* along the R^1-R^2 direction onto a perpendicular plane passing through the metal atom.



Scheme S1. Definitions of angles ϕ, θ_i, and ω_{ij} for metal coordination spheres in (a) *fac*-[Os(**L1**)$_3$]$^{2+}$ and (b) *mer*-[Os(**L1**)$_3$]$^{2+}$.

Table S2. Selected geometric parameters[a] for *HHH*-[OsLu(**L2**)$_3$]$^{5+}$ (**3**) and *HHH*-[RuLu(**L2**)$_3$]$^{5+}$ (values listed in parentheses).

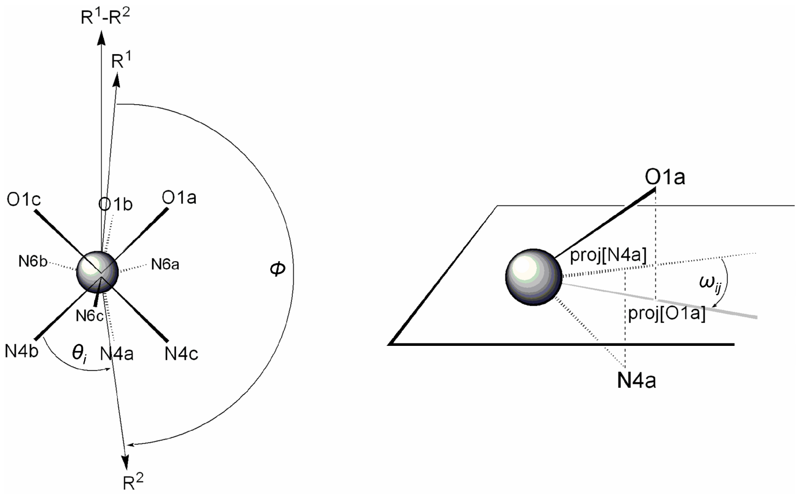
	Os coordination sphere		
Angles ϕ (°)			
R^1-Os-R^2 [b]	179.3 (178.5)		
Angles θ_i (°)			
R^1-Os-N2a	57.67 (62.0)	R^2-Os-N1a	65.99 (60.2)
R^1-Os-N2b	60.15 (61.1)	R^2-Os-N1b	57.16 (59.1)
R^1-Os-N2c	67.86 (62.0)	R^2-Os-N1c	58.21 (60.6)
Angles ω_{ij} (°) (intra-)			
proj[N2a]-Os-proj[N1a][c]	44.28 (54.5)		
proj[N2b]-Os-proj[N1b]	64.53 (52.9)		
proj[N2c]-Os-proj[N1c]	51.45 (54.1)		
Angles ω_{ij} (°) (inter-)			
proj[N2a]-Os-proj[N2b]	110.03 (119.4)		
proj[N2a]-Os-proj[N2c]	126.67 (120.8)		
proj[N2b]-Os-proj[N2c]	123.30 (119.8)		
proj[N1a]-Os-proj[N1b]	125.81 (117.7)		
proj[N1a]-Os-proj[N1c]	123.86 (121.3)		
proj[N1b]-Os-proj[N1c]	110.33 (121.0)		
proj[N2a]-Os-proj[N1b]	170.06 (172.3)		
proj[N2a]-Os-proj[N1c]	79.59 (66.7)		
proj[N2b]-Os-proj[N1a]	61.47 (64.9)		
proj[N2b]-Os-proj[N1c]	172.99 (173.9)		
proj[N2c]-Os-proj[N1a]	173.57 (175.3)		
proj[N2c]-Os-proj[N1b]	59.10 (67.0)		

[a] For definitions of ϕ, θ_i, and ω_{ij} see Scheme S1 (the error is in the range 1-2 °). [b] Vectors R^i are as defined as follows: R^1 = Os-N2a + Os-N2b + Os-N2c and R^2 = Os-N1a + Os-N1b + Os-N1c. [c] Proj[N*i*] is the projection of N*i* along the R^1-R^2 direction onto a perpendicular plane passing through the metal atom.

Table S2. (cont.)

	Lu coordination sphere[a]		
Angles ϕ (°)			
R[1]-Lu-R[2] [b]	177.8 (177.6)		
Angles θ_i (°)			
R^1-Lu-O1a	47.85 (46.4)	R^2-Lu-N4a	49.97 (52.4)
R^1-Lu-O1b	52.45 (46.6)	R^2-Lu-N4b	60.34 (48.8)
R^1-Lu-O1c	44.12 (46.9)	R^2-Lu-N4c	46.52 (52.5)
Angles ω_{ij} (°) (intra-)			
proj[N4a]-Lu-proj[N6a][c]	41.26 (53.9)	proj[N6b]-Lu-proj[O1b]	61.38 (59.2)
proj[N6a]-Lu-proj[O1a]	67.05 (56.9)	proj[N4c]-Lu-proj[N6c]	54.35 (52.0)
proj[N4b]-Lu-proj[N6b]	60.79 (50.9)	proj[N6c]-Lu-proj[O1c]	45.53 (58.4)
Angles ω_{ij} (°) (inter-)			
proj[N4a]-Lu-proj[O1c]	6.57 (8.9)		
proj[N4c]-Lu-proj[O1b]	11.24 (8.6)		
proj[N4b]-Lu-proj[O1a]	11.84 (11.3)		
proj[N4b]-Lu-proj[N6c]	171.90 (169.8)		
proj[N4a]-Lu-proj[N6b]	174.49 (174.1)		
proj[N4c]-Lu-proj[N6a]	170.01 (172.9)		
proj[N4c]-Lu-proj[N6b]	56.76 (67.0)		
proj[N4b]-Lu-proj[N6a]	78.88 (68.2)		
proj[N4a]-Lu-proj[N6c]	67.95 (68.1)		
proj[N6a]-Lu-proj[N6c]	109.21 (122.0)		
proj[N6b]-Lu-proj[N6c]	117.56 (117.9)		
proj[N6a]-Lu-proj[N6b]	133.23 (120.1)		

[a] For definitions of ϕ, θ_i, and ω_{ij} see Scheme S2 (the error is in the range 1-2 °). [b] Vectors R^i are as defined as follows: R^1 = Lu-O1a + Os-O1b + Os-O1c and R^2 = Os-N4a + Os-N4b + Os-N4c. [c] Proj[N*i*] is the projection of N*i* along the R^1-R^2 direction onto a perpendicular plane passing through the metal atom.

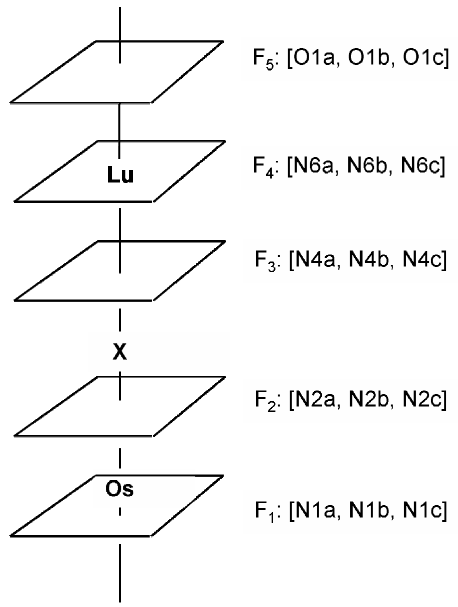


Scheme S2. Definitions of angles ϕ, θ_i and ω_{ij} for the pseudo tricapped trigonal prismatic Lu coordination sphere in *HHH*-$[OsLu(L2)_3]^{5+}$.

Table S3. Helical pitches P_{ij}, linear distances $d(F_i\text{-}F_j)$ and average twist angles α_{ij} along the pseudo-C_3 axis[a] in the crystal structures of *HHH*-[OsLu(**L2**)$_3$]$^{5+}$ (**3**) and *HHH*-[RuLu(**L2**)$_3$]$^{5+}$.[b]

	HHH-[OsLu(**L2**)$_3$]$^{5+}$ (**3**)				*HHH*-[RuLu(**L2**)$_3$]$^{5+}$		
	$d(F_i\text{-}F_j)$ (Å)	α_{ij} (°)[c]	P_{ij} (Å)		$d(F_i\text{-}F_j)$ (Å)	α_{ij} (°)	P_{ij} (Å)
F_1-F_2[d]	1.99	53	13.43	F_1-F_2	2.00	54	13.35
F_2-F_3	6.60	117	20.18	F_2-F_3	6.46	117	19.86
F_3-F_4	1.51	52	10.39	F_3-F_4	1.75	52	12.06
F_4-F_5	1.53	59	9.30	F_4-F_5	1.41	58	8.72
F_1-F_5	11.64	282	13.33	F_1-F_5	11.62	281	14.88
Os···Lu	9.0885(8)	-	-	Ru···Lu	9.0794(9)	-	-

[a] Each helical portion F_1-F_2, F_2-F_3, F_3-F_4 and F_4-F_5 is characterised by 1) a linear extension $d(F_i\text{-}F_j)$ defined by the separation between the facial planes, 2) an average twist angle α_{ij} defined by the angular rotation between the projections of N_i and N_j (or O_j) belonging to the same ligand strand onto an intermediate plane passing through the metal (or the midpoint X in Scheme S3) and 3) its pitch P_{ij} defined as the ratio of axial over angular progressions along the helical axis $P_{ij} = d(F_i\text{-}F_j)/(\alpha_{ij}/360)$ (P_{ij} corresponds to the length of a cylinder containing a single turn of the helix defined by geometrical characteristics $d(F_i\text{-}F_j)$ and α_{ij}). [b] Taken from ref. 10b. [c] α_{ij} are given as C_3 average values. [d] F_1: N1a, N1b, N1c; F_2: N2a, N2b, N2c; F_3: N4a, N4b, N4c; F_4: N6a, N6b, N6c; F_5: O1a, O1b, O1c (see Scheme S3).



Scheme S3. Helical portions F_i-F_j.

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H22c .42660 .28169 .85694 .05000 1.00000 Uiso
H23c .35732 .18409 .91060 .05000 1.00000 Uiso
H24c .41138 .06744 .86598 .05000 1.00000 Uiso
H271c .63301 -.06927 .72094 .05000 1.00000 Uiso
H272c .61335 -.13634 .78238 .05000 1.00000 Uiso
H281c .49965 -.11480 .73251 .05000 1.00000 Uiso
H282c .51931 -.04773 .67106 .05000 1.00000 Uiso

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H283c .57143 -.13414 .67103 .05000 1.00000 Uiso
H291c .45572 -.01895 .89013 .05000 1.00000 Uiso
H292c .50193 -.10687 .88636 .05000 1.00000 Uiso
H301c .61530 -.09816 .91498 .05000 1.00000 Uiso
H302c .56909 -.01024 .91874 .05000 1.00000 Uiso
H303c .53942 -.07589 .97463 .05000 1.00000 Uiso
H311c 1.07288 .34486 1.07502 .05000 1.00000 Uiso
H312c 1.12728 .25838 1.07949 .05000 1.00000 Uiso
H313c 1.16818 .32271 1.05950 .05000 1.00000 Uiso
H321c 1.20591 .29524 .61647 .05000 1.00000 Uiso
H322c 1.22957 .33385 .67095 .05000 1.00000 Uiso
H323c 1.22833 .24768 .69632 .05000 1.00000 Uiso
H331c .47045 .44702 .75216 .05000 1.00000 Uiso
H332c .44084 .39080 .72386 .05000 1.00000 Uiso
H333c .46341 .36992 .80532 .05000 1.00000 Uiso
H11i 1.08718 .09500 .96967 .05000 1.00000 Uiso
H12i 1.08060 .14102 1.03145 .05000 1.00000 Uiso
H13i 1.06469 .18677 .94947 .05000 1.00000 Uiso
H21j .40658 .61642 .95297 .05000 1.00000 Uiso
H23j .43807 .52519 .97737 .05000 1.00000 Uiso
H22j .34924 .56815 .95293 .05000 1.00000 Uiso
H22k .54886 .72510 .84225 .05000 1.00000 Uiso
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H23k .54470 .65897 .80619 .05000 1.00000 Uiso


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_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Lu .0176(3) .01309(18) .0323(4) -.00007(16) -.0089(3) -.00429(19)
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Os .0205(3) .00941(16) .0324(4) -.00119(14) -.0111(3) -.00052(17)

O1a .023(4) .028(4) .029(5) .006(3) -.019(4) -.011(4)

N1a .037(5) .013(3) .025(6) -.005(3) -.025(4) -.003(3)

N2a .023(5) .008(3) .039(7) .000(3) -.020(4) -.005(4)

N3a .035(5) .011(3) .038(7) -.000(3) -.022(5) .002(4)

N4a .017(4) .012(3) .045(7) .006(3) -.014(4) -.006(4)

N5a .019(5) .016(4) .050(7) .005(3) -.016(5) -.006(4)

N6a .030(5) .010(3) .045(7) .005(3) -.022(5) -.012(4)

N7a .029(5) .021(4) .056(8) .017(4) -.030(5) -.012(4)

C1a .032(6) .011(4) .048(9) .004(4) -.021(6) .004(4)

C2a .029(6) .024(4) .029(8) .001(4) -.017(5) -.005(5)

C3a .043(7) .030(5) .045(9) -.001(5) -.013(6) -.010(5)

C4a .045(7) .017(4) .041(8) -.004(4) -.026(6) -.001(5)

C5a .032(6) .013(4) .044(8) -.004(4) -.019(6) -.002(4)

C6a .024(6) .019(4) .031(8) -.002(4) -.019(5) -.002(4)

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C8a .031(6) .014(4) .050(9) -.003(4) -.028(6) .001(5)

C9a .022(5) .017(4) .063(9) .004(4) -.024(6) -.010(5)

C10a .042(7) .012(4) .062(10) -.004(4) -.025(7) -.005(5)

C11a .043(6) .010(4) .039(8) .000(4) -.024(6) -.002(4)

C12a .028(6) .016(4) .054(9) .001(4) -.026(6) -.005(5)

C13a .028(6) .016(4) .045(8) .002(4) -.019(6) -.007(5)

C14a .033(6) .008(4) .053(9) .006(4) -.025(6) -.016(4)

C15a .015(5) .012(4) .037(8) .003(4) -.011(5) -.006(4)

C16a .030(6) .015(4) .036(8) .001(4) -.018(5) -.009(4)

C17a .036(6) .018(4) .027(7) -.002(4) -.017(5) .002(4)

C18a .018(5) .023(4) .051(9) -.007(4) -.013(5) -.003(5)

C19a .023(6) .019(4) .061(9) -.001(4) -.024(6) -.004(5)

C20a .027(6) .012(4) .039(8) .001(4) -.011(5) -.008(4)

C21a .025(6) .015(4) .036(8) -.003(4) -.015(5) -.007(4)

C22a .034(6) .013(4) .035(8) -.004(4) -.009(6) .004(4)

C23a .044(7) .019(4) .044(8) -.010(5) -.018(6) -.005(5)

C24a .035(6) .020(4) .045(9) -.002(4) -.023(6) -.004(5)

C25a .026(6) .013(4) .044(8) -.004(4) -.017(6) -.008(4)

C26a .031(6) .016(4) .037(8) .002(4) -.015(6) -.004(5)

C27a	.039(7)	.016(5)	.109(13)	.012(5)	-.039(8)	-.010(6)
C28a	.088(11)	.039(6)	.135(17)	.004(7)	-.093(11)	.016(8)
C29a	.025(6)	.042(6)	.062(10)	.016(5)	-.015(6)	-.021(6)
C30a	.022(6)	.036(5)	.055(10)	.005(5)	-.016(6)	-.005(6)
C31a	.057(8)	.022(5)	.039(8)	.004(5)	-.023(7)	-.006(5)
C32a	.067(8)	.011(4)	.047(9)	-.003(5)	-.017(7)	.007(5)
C33a	.024(6)	.020(4)	.071(10)	-.009(4)	-.014(6)	.001(5)
O1b	.033(4)	.013(3)	.039(5)	.005(3)	-.013(4)	-.009(3)
N1b	.017(4)	.013(3)	.031(6)	.006(3)	-.011(4)	-.008(4)
N2b	.022(5)	.021(4)	.018(6)	.000(3)	-.016(4)	.005(4)
N3b	.031(5)	.016(4)	.042(7)	.011(4)	-.026(5)	-.003(4)
N4b	.016(4)	.021(4)	.040(7)	-.001(3)	-.012(4)	-.000(4)
N5b	.036(5)	.017(4)	.044(7)	.002(4)	-.028(5)	-.002(4)
N6b	.024(5)	.019(4)	.039(7)	-.001(3)	-.022(5)	-.002(4)
N7b	.041(6)	.021(4)	.040(7)	.008(4)	-.025(5)	-.012(4)
C1b	.025(6)	.017(4)	.039(8)	-.003(4)	-.011(5)	-.003(4)
C2b	.039(7)	.017(4)	.036(8)	-.007(4)	-.009(6)	-.006(4)
C3b	.041(7)	.012(4)	.042(8)	.001(4)	-.011(6)	.004(4)
C4b	.036(6)	.012(4)	.032(8)	.001(4)	-.006(6)	.003(4)
C5b	.032(6)	.017(4)	.021(7)	.000(4)	-.010(5)	-.001(4)
C6b	.028(6)	.011(4)	.025(7)	.005(4)	-.017(5)	-.002(4)
C7b	.035(6)	.029(5)	.015(7)	.000(4)	-.011(5)	-.006(4)
C8b	.032(6)	.016(4)	.034(8)	-.000(4)	-.019(5)	-.004(4)
C9b	.035(6)	.027(5)	.024(7)	-.008(4)	-.015(5)	-.006(5)
C10b	.028(6)	.034(5)	.050(9)	-.003(5)	-.017(6)	-.009(5)
C11b	.025(6)	.031(5)	.052(9)	.006(4)	-.021(6)	-.017(5)
C12b	.026(6)	.025(5)	.025(7)	.005(4)	-.012(5)	-.006(5)
C13b	.028(6)	.031(5)	.046(9)	-.005(5)	-.011(6)	-.007(5)
C14b	.029(6)	.023(5)	.041(9)	-.008(4)	-.010(6)	-.003(5)
C15b	.035(6)	.019(4)	.039(9)	-.004(4)	-.019(6)	.001(5)
C16b	.021(5)	.021(4)	.039(8)	-.006(4)	-.015(5)	.003(5)
C17b	.028(6)	.023(5)	.042(9)	-.010(4)	-.016(6)	.001(5)
C18b	.029(6)	.028(5)	.061(10)	-.006(5)	-.024(6)	.002(5)
C19b	.037(7)	.034(5)	.033(8)	-.013(5)	-.016(6)	.004(5)
C20b	.018(5)	.015(4)	.056(10)	-.000(4)	-.015(6)	.001(5)

C21b	.020(6)	.026(5)	.056(9)	.002(4)	-.013(6)	-.009(5)
C22b	.057(8)	.021(5)	.070(11)	.018(5)	-.043(8)	-.006(6)
C23b	.061(9)	.024(5)	.075(11)	.023(5)	-.044(8)	-.022(6)
C24b	.038(7)	.034(5)	.066(11)	.010(5)	-.030(7)	-.015(6)
C25b	.034(6)	.022(4)	.034(8)	-.003(4)	-.014(6)	-.009(5)
C26b	.028(6)	.023(5)	.030(8)	-.002(4)	-.007(5)	-.008(5)
C27b	.067(9)	.027(5)	.077(11)	.006(6)	-.042(8)	-.019(6)
C28b	.064(9)	.029(6)	.087(13)	-.007(6)	-.027(9)	.002(7)
C29b	.050(8)	.039(6)	.051(10)	.005(5)	-.034(7)	-.014(6)
C30b	.063(10)	.057(8)	.151(18)	.027(7)	-.072(11)	-.042(9)
C31b	.035(7)	.024(5)	.063(10)	-.012(5)	-.012(6)	.001(5)
C32b	.044(7)	.016(4)	.066(10)	.011(4)	-.036(7)	.005(5)
C33b	.050(7)	.018(4)	.066(10)	.008(5)	-.029(7)	.009(5)
O1c	.021(4)	.019(3)	.042(6)	.002(3)	-.012(4)	-.008(3)
N1c	.039(5)	.014(3)	.012(6)	-.001(3)	-.020(5)	-.002(3)
N2c	.022(5)	.015(3)	.039(7)	.001(3)	-.018(4)	-.009(4)
N3c	.029(5)	.018(4)	.030(7)	.002(4)	-.013(5)	-.002(4)
N4c	.030(5)	.015(3)	.038(6)	.002(3)	-.020(5)	-.004(4)
N5c	.029(5)	.013(3)	.041(7)	.008(3)	-.013(5)	-.010(4)
N6c	.023(5)	.021(4)	.032(6)	.006(4)	-.017(4)	-.009(4)
N7c	.034(5)	.019(4)	.052(8)	.001(4)	-.015(5)	-.003(4)
C1c	.031(6)	.016(4)	.050(9)	-.005(4)	-.014(6)	-.006(5)
C2c	.028(6)	.028(5)	.064(10)	.001(5)	-.018(7)	-.009(6)
C3c	.035(7)	.036(6)	.049(10)	.002(5)	-.031(7)	-.005(6)
C4c	.029(6)	.024(5)	.068(11)	.001(4)	-.014(7)	-.004(5)
C5c	.029(6)	.010(4)	.042(8)	-.005(4)	-.011(6)	-.003(4)
C6c	.028(6)	.016(4)	.038(8)	-.005(4)	-.010(6)	.000(4)
C7c	.034(6)	.011(4)	.040(8)	-.008(4)	-.010(6)	-.002(4)
C8c	.023(6)	.013(4)	.033(8)	-.001(4)	-.017(5)	-.003(4)
C9c	.028(6)	.014(4)	.043(9)	-.005(4)	-.014(6)	.003(5)
C10c	.041(7)	.027(5)	.038(8)	-.008(5)	-.013(6)	.006(5)
C11c	.033(6)	.024(5)	.041(9)	-.004(4)	-.003(6)	-.013(5)
C12c	.024(6)	.016(4)	.039(8)	-.004(4)	-.003(6)	-.006(4)
C13c	.042(7)	.019(4)	.029(7)	-.006(4)	-.024(6)	.001(4)
C14c	.037(6)	.022(4)	.030(7)	-.003(4)	-.019(6)	-.003(4)

C15c .023(5) .023(4) .028(7) -.005(4) -.010(5) -.009(4)

C16c .035(6) .016(4) .038(8) .003(4) -.022(6) .000(4)

C17c .036(6) .023(5) .024(7) .002(4) -.014(6) -.005(4)

C18c .038(7) .013(4) .049(9) -.002(4) -.018(6) -.010(5)

C19c .036(6) .012(4) .040(8) -.000(4) -.017(6) -.003(4)

C20c .029(6) .020(4) .030(7) -.001(4) -.011(5) -.005(4)

C21c .026(6) .016(4) .052(9) .004(4) -.021(6) -.008(5)

C22c .036(7) .029(5) .038(8) -.002(5) -.012(6) -.011(5)

C23c .029(7) .052(6) .047(9) -.004(5) .003(6) -.024(6)

C24c .028(6) .026(5) .063(10) -.008(5) -.006(6) -.014(5)

C25c .027(6) .016(4) .041(8) -.000(4) -.020(5) -.008(4)

C26c .025(6) .020(4) .048(9) -.002(4) -.020(6) -.006(5)

C27c .045(8) .014(4) .093(12) .001(5) -.018(8) -.016(6)

C28c .060(9) .041(6) .135(17) -.000(6) -.032(10) -.041(8)

C29c .038(7) .028(5) .061(10) -.009(5) -.009(7) -.001(6)

C30c .075(10) .057(7) .054(11) -.020(7) -.029(9) .005(7)

C31c .038(7) .060(7) .054(10) .005(6) -.030(7) -.022(7)

C32c .022(6) .031(5) .056(9) .001(4) -.011(6) -.012(5)

C33c .017(6) .022(4) .065(10) .015(4) -.016(6) -.008(5)

S1d .0338(15) .0205(10) .047(3) .0003(10) -.0147(14) -.0068(11)

O1d .051(5) .037(4) .049(6) .000(4) -.005(5) -.010(4)

O2d .055(5) .021(3) .077(7) .000(4) -.041(5) -.003(4)

O3d .052(5) .033(4) .059(7) .012(4) -.032(5) -.017(4)

C1d .048(8) .028(5) .068(11) .004(5) -.009(7) -.015(6)

F1d .081(6) .034(3) .056(6) .000(4) .005(5) -.012(4)

F2d .055(5) .038(4) .110(8) -.018(4) -.015(5) -.024(4)

F3d .072(5) .016(3) .073(6) .011(3) -.027(5) -.000(3)

S1e .0386(18) .0508(15) .051(3) -.0016(13) -.0137(17) -.0082(15)

O1e .049(6) .121(8) .083(10) -.022(6) -.025(6) -.027(7)

O2e .059(6) .092(6) .070(8) .035(5) -.031(6) -.051(6)

O3e .045(6) .051(5) .068(8) .019(4) -.013(5) -.025(5)

C1e .013(7) .080(10) .26(4) .006(7) -.038(12) -.034(14)

F1e .079(7) .056(5) .243(17) .003(5) -.027(9) -.023(7)

F2e .127(10) .107(8) .166(14) .041(8) .007(11) .047(9)

F3e .068(7) .065(5) .233(15) .033(5) -.036(8) .030(7)

S1f .0419(17) .0252(11) .065(3) -.0056(11) -.0173(17) .0019(13)

O1f .059(6) .031(4) .087(8) -.003(4) -.006(6) -.015(5)

O2f .059(6) .039(4) .086(9) -.001(4) -.047(6) .010(5)

O3f .063(6) .023(4) .076(8) -.003(4) -.021(5) -.013(4)

C1f .044(7) .027(5) .041(9) -.008(5) -.020(6) -.003(5)

F1f .047(5) .048(4) .075(7) .005(4) -.009(5) -.002(4)

F2f .068(5) .038(3) .061(6) .007(3) -.044(5) .003(4)

F3f .086(6) .042(4) .074(7) .007(4) -.039(5) -.026(4)

S1g .050(3) .070(3) .120(5) -.0212(19) .002(3) -.011(3)

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_geom_bond_site_symmetry_2

_geom_bond_distance

Lu O1a . . 2.031(7)

Lu N4a . . 2.788(8)

Lu N6a . . 2.675(8)

Lu O1b . . 2.338(8)

Lu N4b . . 2.269(9)

Lu N6b . . 2.314(7)

Lu O1c . . 2.616(7)

Lu N4c . . 2.517(8)

Lu N6c . . 2.814(8)

Os N1a . . 2.248(9)

Os N2a . . 2.148(7)

Os N1b . . 2.103(7)

Os N2b . . 1.879(8)

Os C6b . . 2.502(8)

Os N1c . . 1.922(9)

Os N2c . . 2.254(9)

O1a C26a . . 1.271(11)

N1a C1a . . 1.312(12)

N1a C5a . . 1.437(11)

N2a C6a . . 1.464(14)

N2a C7a . . 1.363(12)

N3a C6a . . 1.391(11)

N3a C12a . . 1.412(15)

N3a C32a . . 1.633(14)

N4a C16a . . 1.314(14)

N4a C20a . . 1.423(13)

N5a C17a . . 1.261(14)

N5a C20a . . 1.498(13)

N5a C33a . . 1.696(14)

N6a C21a . . 1.512(13)

N6a C25a . . 1.178(14)

N7a C26a . . 1.184(11)

N7a C27a . . 1.445(12)

N7a C29a . . 1.738(15)

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C18a C19a . . 1.332(16)

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C27a C28a . . 1.42(3)

C29a C30a . . 1.519(19)

O1b C26b . . 1.228(11)

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N1b C5b . . 1.220(12)

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N2b C7b . . 1.504(14)

N3b C6b . . 1.288(13)

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N4b C16b . . 1.428(16)

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N5b C17b . . 1.393(14)

N5b C20b . . 1.296(15)

N5b C33b . . 1.337(10)

N6b C21b . . 1.213(14)

N6b C25b . . 1.367(16)

N7b C26b . . 1.256(17)

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N7b C29b . . 1.329(14)

C1b C2b . . 1.412(12)

C2b C3b . . 1.194(15)

C2b C31b . . 1.635(17)

C3b C4b . . 1.490(17)

C4b C5b . . 1.419(12)

C5b C6b . . 1.573(15)

C7b C8b . . 1.511(13)

C7b C12b . . 1.229(12)

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C14b C15b . . 1.366(18)

C14b C19b . . 1.311(13)

C15b C16b . . 1.378(14)

C16b C17b . . 1.253(12)

C17b C18b . . 1.446(19)

C18b C19b . . 1.339(15)

C20b C21b . . 1.493(18)

C21b C22b . . 1.307(13)

C22b C23b . . 1.44(3)

C23b C24b . . 1.209(19)

C24b C25b . . 1.303(13)

C25b C26b . . 1.313(14)

C27b C28b . . 1.55(3)

C29b C30b . . 1.601(19)

O1c C26c . . 1.411(13)

N1c C1c . . 1.261(16)

N1c C5c . . 1.505(13)

N2c C6c . . 1.302(13)

N2c C7c . . 1.359(16)

N3c C6c . . 1.494(14)

N3c C12c . . 1.211(15)

N3c C32c . . 1.488(13)

N4c C16c . . 1.522(13)

N4c C20c . . 1.419(12)

N5c C17c . . 1.583(14)

N5c C20c . . 1.280(10)

N5c C33c . . 1.424(12)

N6c C21c . . 1.292(12)

N6c C25c . . 1.492(13)

N7c C26c . . 1.373(12)

N7c C27c . . 1.495(16)

N7c C29c . . 1.610(16)

C1c C2c . . 1.288(16)

C2c C3c . . 1.518(17)

C2c C31c . . 1.47(3)

C3c C4c . . 1.32(3)

C4c C5c . . 1.341(16)

C5c C6c . . 1.366(18)

C7c C8c . . 1.239(15)

C7c C12c . . 1.546(14)

C8c C9c . . 1.406(16)

C9c C10c . . 1.544(15)

C9c C13c . . 1.356(15)

C10c C11c . . 1.218(16)

C11c C12c . . 1.425(17)

C13c C14c . . 1.738(15)

C14c C15c . . 1.464(13)

C14c C19c . . 1.294(12)

C15c C16c . . 1.573(14)

C16c C17c . . 1.304(12)

C17c C18c . . 1.462(14)

C18c C19c . . 1.550(15)

C20c C21c . . 1.666(14)

C21c C22c . . 1.542(15)

C22c C23c . . 1.537(17)

C23c C24c . . 1.338(16)

C24c C25c . . 1.527(15)

C25c C26c . . 1.467(14)

C27c C28c . . 1.44(3)

C29c C30c . . 1.39(3)

S1d O1d . . 1.498(9)

S1d O2d . . 1.447(11)

S1d O3d . . 1.281(8)

S1d C1d . . 2.026(12)

C1d F1d . . 1.418(16)

C1d F2d . . 1.363(18)

C1d F3d . . 1.152(12)

S1e O1e . . 1.436(14)

S1e O2e . . 1.490(12)

S1e O3e . . 1.407(8)

S1e C1e . . 1.719(18)

C1e F1e . . 1.35(3)

C1e F2e . . 1.62(4)

C1e F3e . . 1.183(15)

S1f O1f . . 1.685(9)

S1f O2f . . 1.399(11)

S1f O3f . . 1.462(11)

S1f C1f . . 1.698(10)

C1f F1f . . 1.529(14)

C1f F2f . . 1.255(14)

C1f F3f . . 1.345(16)

S1g O1g . . 1.407(16)

S1g O2g . . 1.271(13)

S1g O3g . . 1.616(19)

S1g C1g . . 1.781(16)

C1g F1g . . 1.157(19)

C1g F2g . . 1.30(3)

C1g F3g . . 1.637(16)

S1g O1g' . . 1.60(3)

S1g O2g' . . 1.29(3)

S1g O3g' . . 1.48(3)

S1g C1g' . . 1.932(16)

C1g' F1g' . . 1.113(15)

C1g' F2g' . . 1.47(3)

C1g' F3g' . . 1.35(3)

S1h O1h . . 1.39(2)

S1h O2h . . 1.505(13)

S1h O3h . . 1.572(18)

S1h C1h . . 1.649(15)

C1h F1h . . 1.37(3)
C1h F2h . . 1.264(16)
C1h F3h . . 1.50(3)
S1h' O1h' . . 1.50(3)
S1h' O2h' . . 1.591(17)
S1h' O3h' . . 1.322(14)
S1h' C1h' . . 1.729(15)
C1h' F1h' . . 1.178(16)
C1h' F2h' . . 1.56(3)
C1h' F3h' . . 1.38(2)
O1i C1i . . 1.441(16)
N1j C1j . . 1.22(3)
C1j C2j . . 1.46(3)
N1k C1k . . 1.10(4)
C1k C2k . . 1.44(4)

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle
O1a Lu N4a . . . 127.4(3)
O1a Lu N6a . . . 76.9(3)
O1a Lu O1b . . . 80.9(3)
O1a Lu N4b . . . 133.2(3)
O1a Lu N6b . . . 125.8(4)
O1a Lu O1c . . . 73.8(3)
O1a Lu N4c . . . 84.1(3)
O1a Lu N6c . . . 67.5(3)
N4a Lu N6a . . . 50.6(3)
N4a Lu O1b . . . 79.1(3)

N4a Lu N4b . . . 94.9(3)

N4a Lu N6b . . . 82.5(3)

N4a Lu O1c . . . 150.73(17)

N4a Lu N4c . . . 80.9(3)

N4a Lu N6c . . . 146.1(3)

N6a Lu O1b . . . 62.5(3)

N6a Lu N4b . . . 142.9(3)

N6a Lu N6b . . . 110.0(3)

N6a Lu O1c . . . 139.8(3)

N6a Lu N4c . . . 77.9(3)

N6a Lu N6c . . . 133.54(19)

O1b Lu N4b . . . 132.2(3)

O1b Lu N6b . . . 59.6(3)

O1b Lu O1c . . . 86.0(3)

O1b Lu N4c . . . 139.8(3)

O1b Lu N6c . . . 134.7(3)

N4b Lu N6b . . . 72.6(3)

N4b Lu O1c . . . 76.7(3)

N4b Lu N4c . . . 83.9(3)

N4b Lu N6c . . . 65.8(3)

N6b Lu O1c . . . 68.2(3)

N6b Lu N4c . . . 149.8(3)

N6b Lu N6c . . . 114.8(3)

O1c Lu N4c . . . 125.0(3)

O1c Lu N6c . . . 55.1(3)

N4c Lu N6c . . . 69.9(3)

N1a Os N2a . . . 69.1(3)

N1a Os N1b . . . 105.8(3)

N1a Os N2b . . . 80.8(4)

N1a Os C6b . . . 90.1(3)

N1a Os N1c . . . 102.8(4)

N1a Os N2c . . . 174.1(3)

N2a Os N1b . . . 174.2(3)

N2a Os N2b . . . 86.0(3)

N2a Os C6b . . . 116.4(3)

N2a Os N1c . . . 99.1(3)

N2a Os N2c . . . 108.4(3)

N1b Os N2b . . . 90.3(3)

N1b Os C6b . . . 59.8(3)

N1b Os N1c . . . 84.8(3)

N1b Os N2c . . . 76.9(3)

N2b Os C6b . . . 30.5(3)

N2b Os N1c . . . 174.6(3)

N2b Os N2c . . . 104.6(4)

C6b Os N1c . . . 144.5(3)

C6b Os N2c . . . 95.8(3)

N1c Os N2c . . . 72.0(4)

C1a N1a C5a . . . 111.6(9)

C6a N2a C7a . . . 103.6(7)

C6a N3a C12a . . . 98.2(8)

C6a N3a C32a . . . 131.2(9)

C12a N3a C32a . . . 130.5(7)

C16a N4a C20a . . . 93.5(8)

C17a N5a C20a . . . 94.1(8)

C17a N5a C33a . . . 125.2(9)

C20a N5a C33a . . . 140.6(8)

C21a N6a C25a . . . 115.0(10)

C26a N7a C27a . . . 111.9(9)

C26a N7a C29a . . . 119.7(8)

C27a N7a C29a . . . 127.5(7)

N1a C1a C2a . . . 123.4(8)

C1a C2a C3a . . . 124.4(9)

C1a C2a C31a . . . 117.9(8)

C3a C2a C31a . . . 117.6(10)

C2a C3a C4a . . . 114.4(11)

C3a C4a C5a . . . 118.4(9)

N1a C5a C4a . . . 127.7(8)

N1a C5a C6a . . . 106.0(9)

C4a C5a C6a . . . 126.2(8)

N2a C6a N3a . . . 117.6(9)

N2a C6a C5a . . . 117.5(8)

N3a C6a C5a . . . 124.9(10)

N2a C7a C8a . . . 126.0(8)

N2a C7a C12a . . . 106.1(9)

C8a C7a C12a . . . 127.9(8)

C7a C8a C9a . . . 112.6(9)

C8a C9a C10a . . . 119.1(11)

C8a C9a C13a . . . 115.8(9)

C10a C9a C13a . . . 125.0(8)

C9a C10a C11a . . . 128.2(9)

C10a C11a C12a . . . 111.7(9)

N3a C12a C7a . . . 114.4(8)

N3a C12a C11a . . . 125.1(9)

C7a C12a C11a . . . 120.4(10)

C9a C13a C14a . . . 124.7(7)

C13a C14a C15a . . . 105.4(9)

C13a C14a C19a . . . 126.4(10)

C15a C14a C19a . . . 128.2(10)

C14a C15a C16a . . . 103.4(9)

N4a C16a C15a . . . 120.1(10)

N4a C16a C17a . . . 112.4(9)

C15a C16a C17a . . . 127.6(10)

N5a C17a C16a . . . 112.5(9)

N5a C17a C18a . . . 117.0(10)

C16a C17a C18a . . . 130.5(10)

C17a C18a C19a . . . 100.6(9)

C14a C19a C18a . . . 129.7(10)

N4a C20a N5a . . . 127.4(9)

N4a C20a C21a . . . 114.0(9)

N5a C20a C21a . . . 118.6(9)

N6a C21a C20a . . . 105.8(9)

N6a C21a C22a . . . 134.1(10)

C20a C21a C22a . . . 120.1(10)

C21a C22a C23a . . . 110.8(10)

C22a C23a C24a . . . 114.5(11)

C23a C24a C25a . . . 131.7(10)

N6a C25a C24a . . . 113.7(9)

N6a C25a C26a . . . 110.3(9)

C24a C25a C26a . . . 135.4(10)

O1a C26a N7a . . . 107.5(9)

O1a C26a C25a . . . 127.9(7)

N7a C26a C25a . . . 124.5(8)

N7a C27a C28a . . . 104.6(11)

N7a C29a C30a . . . 116.7(10)

C1b N1b C5b . . . 117.7(7)

C6b N2b C7b . . . 119.6(8)

C6b N3b C12b . . . 120.0(7)

C6b N3b C32b . . . 113.9(9)

C12b N3b C32b . . . 126.1(9)

C16b N4b C20b . . . 108.5(9)

C17b N5b C20b . . . 115.3(7)

C17b N5b C33b . . . 119.4(10)

C20b N5b C33b . . . 124.9(10)

C21b N6b C25b . . . 124.5(8)

C26b N7b C27b . . . 132.2(9)

C26b N7b C29b . . . 116.0(9)

C27b N7b C29b . . . 111.8(11)

N1b C1b C2b . . . 133.8(8)

C1b C2b C3b . . . 108.3(11)

C1b C2b C31b . . . 130.1(9)

C3b C2b C31b . . . 121.5(9)

C2b C3b C4b . . . 118.8(9)

C3b C4b C5b . . . 133.1(9)

N1b C5b C4b . . . 108.1(10)

N1b C5b C6b . . . 111.8(7)

C4b C5b C6b . . . 139.7(9)

N2b C6b N3b . . . 94.8(8)

N2b C6b C5b . . . 127.7(8)

N3b C6b C5b . . . 137.6(7)

N2b C7b C8b . . . 141.9(8)

N2b C7b C12b . . . 105.4(9)

C8b C7b C12b . . . 112.7(10)

C7b C8b C9b . . . 132.3(8)

C8b C9b C10b . . . 111.5(9)

C8b C9b C13b . . . 132.5(8)

C10b C9b C13b . . . 116.0(10)

C9b C10b C11b . . . 117.2(11)

C10b C11b C12b . . . 130.9(8)

N3b C12b C7b . . . 100.0(10)

N3b C12b C11b . . . 144.4(7)

C7b C12b C11b . . . 115.3(9)

C9b C13b C14b . . . 104.5(9)

C13b C14b C15b . . . 127.3(8)

C13b C14b C19b . . . 110.8(11)

C15b C14b C19b . . . 121.9(10)

C14b C15b C16b . . . 125.2(8)

N4b C16b C15b . . . 135.4(8)

N4b C16b C17b . . . 111.4(9)

C15b C16b C17b . . . 113.0(12)

N5b C17b C16b . . . 99.3(10)

N5b C17b C18b . . . 138.0(8)

C16b C17b C18b . . . 122.8(10)

C17b C18b C19b . . . 123.0(9)

C14b C19b C18b . . . 113.9(12)

N4b C20b N5b . . . 105.5(11)

N4b C20b C21b . . . 120.6(10)

N5b C20b C21b . . . 133.9(7)

N6b C21b C20b . . . 118.7(8)

N6b C21b C22b . . . 109.3(12)

C20b C21b C22b . . . 132.0(11)

C21b C22b C23b . . . 125.3(12)

C22b C23b C24b . . . 123.2(11)

C23b C24b C25b . . . 108.9(14)

N6b C25b C24b . . . 128.3(11)

N6b C25b C26b . . . 113.1(8)

C24b C25b C26b . . . 118.5(12)

O1b C26b N7b . . . 128.6(9)

O1b C26b C25b . . . 106.8(11)

N7b C26b C25b . . . 124.5(9)

N7b C27b C28b . . . 119.4(9)

N7b C29b C30b . . . 99.4(10)

C1c N1c C5c . . . 125.0(9)

C6c N2c C7c . . . 94.3(9)

C6c N3c C12c . . . 108.6(9)

C6c N3c C32c . . . 135.0(9)

C12c N3c C32c . . . 116.3(10)

C16c N4c C20c . . . 117.9(7)

C17c N5c C20c . . . 114.8(7)

C17c N5c C33c . . . 129.7(7)

C20c N5c C33c . . . 115.5(9)

C21c N6c C25c . . . 116.2(8)

C26c N7c C27c . . . 106.5(9)

C26c N7c C29c . . . 131.7(9)

C27c N7c C29c . . . 121.5(8)

N1c C1c C2c . . . 118.2(11)

C1c C2c C3c . . . 117.0(13)

C1c C2c C31c . . . 112.6(11)

C3c C2c C31c . . . 130.3(11)

C2c C3c C4c . . . 127.8(12)

C3c C4c C5c . . . 111.3(11)

N1c C5c C4c . . . 120.5(12)

N1c C5c C6c . . . 118.8(9)

C4c C5c C6c . . . 120.6(11)

N2c C6c N3c . . . 118.5(11)

N2c C6c C5c . . . 106.9(10)

N3c C6c C5c . . . 134.4(10)

N2c C7c C8c . . . 124.2(10)

N2c C7c C12c . . . 118.8(9)

C8c C7c C12c . . . 116.9(11)

C7c C8c C9c . . . 111.4(10)

C8c C9c C10c . . . 130.9(10)

C8c C9c C13c . . . 116.0(9)

C10c C9c C13c . . . 112.8(10)

C9c C10c C11c . . . 119.1(11)

C10c C11c C12c . . . 109.9(10)

N3c C12c C7c . . . 99.7(10)

N3c C12c C11c . . . 128.4(10)

C7c C12c C11c . . . 131.8(10)

C9c C13c C14c . . . 112.1(8)

C13c C14c C15c . . . 131.3(7)

C13c C14c C19c . . . 119.2(8)

C15c C14c C19c . . . 109.3(9)

C14c C15c C16c . . . 129.9(7)

N4c C16c C15c . . . 140.7(7)

N4c C16c C17c . . . 100.2(9)

C15c C16c C17c . . . 119.1(9)

N5c C17c C16c . . . 107.8(8)

N5c C17c C18c . . . 141.0(8)

C16c C17c C18c . . . 111.2(10)

C17c C18c C19c . . . 128.6(8)

C14c C19c C18c . . . 121.9(8)

N4c C20c N5c . . . 99.2(8)

N4c C20c C21c . . . 130.5(7)

N5c C20c C21c . . . 130.2(8)

N6c C21c C20c . . . 110.5(8)

N6c C21c C22c . . . 115.4(9)

C20c C21c C22c . . . 134.0(8)

C21c C22c C23c . . . 128.2(9)

C22c C23c C24c . . . 115.0(10)

C23c C24c C25c . . . 114.1(10)

N6c C25c C24c . . . 130.6(8)

N6c C25c C26c . . . 104.1(8)

C24c C25c C26c . . . 124.9(9)

O1c C26c N7c . . . 128.6(9)

O1c C26c C25c . . . 116.6(8)

N7c C26c C25c . . . 114.9(10)

N7c C27c C28c . . . 117.5(10)

N7c C29c C30c . . . 106.1(10)

O1d S1d O2d . . . 111.8(5)

O1d S1d O3d . . . 116.6(6)

O1d S1d C1d . . . 111.6(5)

O2d S1d O3d . . . 113.6(5)

O2d S1d C1d . . . 110.8(6)

O3d S1d C1d . . . 90.7(5)

S1d C1d F1d . . . 118.1(8)

S1d C1d F2d . . . 119.8(10)

S1d C1d F3d . . . 102.0(9)

F1d C1d F2d . . . 102.2(10)

F1d C1d F3d . . . 109.1(12)

F2d C1d F3d . . . 104.7(10)

O1e S1e O2e . . . 107.9(7)

O1e S1e O3e . . . 112.9(7)

O1e S1e C1e . . . 117.1(10)

O2e S1e O3e . . . 123.0(6)

O2e S1e C1e . . . 101.6(11)

O3e S1e C1e . . . 93.7(7)

S1e C1e F1e . . . 128.4(18)

S1e C1e F2e . . . 116.3(15)

S1e C1e F3e . . . 106.4(12)

F1e C1e F2e . . . 89.9(13)

F1e C1e F3e . . . 106.4(17)

F2e C1e F3e . . . 107.6(19)

O1f S1f O2f . . . 121.6(6)

O1f S1f O3f . . . 116.9(6)

O1f S1f C1f . . . 110.5(5)

O2f S1f O3f . . . 110.6(6)

O2f S1f C1f . . . 90.3(6)

O3f S1f C1f . . . 101.7(6)

S1f C1f F1f . . . 116.6(6)

S1f C1f F2f . . . 98.1(8)

S1f C1f F3f . . . 109.3(9)

F1f C1f F2f . . . 115.9(11)

F1f C1f F3f . . . 110.6(9)

F2f C1f F3f . . . 105.2(8)

O1g S1g O2g . . . 108.8(10)

O1g S1g O3g . . . 117.9(10)

O1g S1g C1g . . . 116.8(9)

O2g S1g O3g . . . 107.1(10)

O2g S1g C1g . . . 102.3(10)

O3g S1g C1g . . . 102.6(8)

S1g C1g F1g . . . 106.7(15)

S1g C1g F2g . . . 107.9(11)

S1g C1g F3g . . . 115.6(9)

F1g C1g F2g . . . 110.5(15)

F1g C1g F3g . . . 106.5(13)

F2g C1g F3g . . . 109.6(12)

O1g' S1g O2g' . . . 110.7(13)

O1g' S1g O3g' . . . 105.6(12)

O1g' S1g C1g' . . . 108.4(11)

O2g' S1g O3g' . . . 111.9(17)

O2g' S1g C1g' . . . 111.4(14)

O3g' S1g C1g' . . . 108.6(10)

S1g C1g' F1g' . . . 109.3(11)

S1g C1g' F2g' . . . 111.5(13)

S1g C1g' F3g' . . . 110.1(11)

F1g' C1g' F2g' . . . 106.7(12)

F1g' C1g' F3g' . . . 107.0(17)

F2g' C1g' F3g' . . . 112.0(15)

O1h S1h O2h . . . 109.7(10)

O1h S1h O3h . . . 112.7(12)

O1h S1h C1h . . . 108.9(9)

O2h S1h O3h . . . 118.7(8)

O2h S1h C1h . . . 100.1(9)

O3h S1h C1h . . . 105.6(9)

S1h C1h F1h . . . 111.5(10)

S1h C1h F2h . . . 109.4(12)
S1h C1h F3h . . . 106.6(11)
F1h C1h F2h . . . 108.1(12)
F1h C1h F3h . . . 109.0(14)
F2h C1h F3h . . . 112.3(11)
O1h' S1h' O2h' . . . 116.1(10)
O1h' S1h' O3h' . . . 111.0(11)
O1h' S1h' C1h' . . . 105.2(9)
O2h' S1h' O3h' . . . 112.1(9)
O2h' S1h' C1h' . . . 108.2(9)
O3h' S1h' C1h' . . . 103.0(9)
S1h' C1h' F1h' . . . 106.4(12)
S1h' C1h' F2h' . . . 112.8(12)
S1h' C1h' F3h' . . . 108.8(9)
F1h' C1h' F2h' . . . 108.6(12)
F1h' C1h' F3h' . . . 109.9(15)
F2h' C1h' F3h' . . . 110.3(12)
N1j C1j C2j . . . 179(3)
N1k C1k C2k . . . 175(3)

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
C5a N1a C1a C2a . . . . 1.2(15)
C1a N1a C5a C4a . . . . .0(16)
C1a N1a C5a C6a . . . . 176.4(10)
C7a N2a C6a N3a . . . . -.4(12)

C7a N2a C6a C5a . . . . -177.2(10)

C6a N2a C7a C8a . . . . -179.8(10)

C6a N2a C7a C12a . . . . -.6(10)

C12a N3a C6a N2a . . . . 1.2(11)

C12a N3a C6a C5a . . . . 177.8(11)

C32a N3a C6a N2a . . . . -179.0(10)

C32a N3a C6a C5a . . . . -2.5(18)

C6a N3a C12a C7a . . . . -1.5(11)

C6a N3a C12a C11a . . . . 179.7(11)

C32a N3a C12a C7a . . . . 178.7(10)

C32a N3a C12a C11a . . . . -.1(18)

C20a N4a C16a C15a . . . . 178.8(9)

C20a N4a C16a C17a . . . . -2.5(9)

C16a N4a C20a N5a . . . . 2.4(11)

C16a N4a C20a C21a . . . . -175.8(9)

C20a N5a C17a C16a . . . . -.9(9)

C20a N5a C17a C18a . . . . 179.9(9)

C33a N5a C17a C16a . . . . 176.4(8)

C33a N5a C17a C18a . . . . -2.8(14)

C17a N5a C20a N4a . . . . -.9(12)

C17a N5a C20a C21a . . . . 177.2(10)

C33a N5a C20a N4a . . . . -177.5(10)

C33a N5a C20a C21a . . . . .6(17)

C25a N6a C21a C20a . . . . 179.4(9)

C25a N6a C21a C22a . . . . -3.3(15)

C21a N6a C25a C24a . . . . .4(12)

C21a N6a C25a C26a . . . . 172.7(7)

C27a N7a C26a O1a . . . . 165.4(11)

C27a N7a C26a C25a . . . . -17.6(18)

C29a N7a C26a O1a . . . . -4.6(16)

C29a N7a C26a C25a . . . . 172.5(11)

C26a N7a C27a C28a . . . . 117.2(13)

C29a N7a C27a C28a . . . . -73.8(16)

C26a N7a C29a C30a . . . . -72.1(15)

C27a N7a C29a C30a . . . . 119.7(13)

N1a C1a C2a C3a . . . . -.6(18)

N1a C1a C2a C31a . . . . 177.8(11)

C1a C2a C3a C4a . . . . -1.3(17)

C31a C2a C3a C4a . . . . -179.7(11)

C2a C3a C4a C5a . . . . 2.3(16)

C3a C4a C5a N1a . . . . -2.0(18)

C3a C4a C5a C6a . . . . -177.7(12)

N1a C5a C6a N2a . . . . -1.6(13)

N1a C5a C6a N3a . . . . -178.2(10)

C4a C5a C6a N2a . . . . 174.8(10)

C4a C5a C6a N3a . . . . -1.8(18)

N2a C7a C8a C9a . . . . 178.3(10)

C12a C7a C8a C9a . . . . -.7(16)

N2a C7a C12a N3a . . . . 1.4(12)

N2a C7a C12a C11a . . . . -179.8(10)

C8a C7a C12a N3a . . . . -179.4(10)

C8a C7a C12a C11a . . . . -.6(17)

C7a C8a C9a C10a . . . . 1.5(15)

C7a C8a C9a C13a . . . . -177.1(9)

C8a C9a C10a C11a . . . . -1.4(18)

C13a C9a C10a C11a . . . . 177.0(11)

C8a C9a C13a C14a . . . . -41.4(16)

C10a C9a C13a C14a . . . . 140.2(11)

C9a C10a C11a C12a . . . . .1(17)

C10a C11a C12a N3a . . . . 179.4(10)

C10a C11a C12a C7a . . . . .8(15)

C9a C13a C14a C15a . . . . -65.6(13)

C9a C13a C14a C19a . . . . 117.4(11)

C13a C14a C15a C16a . . . . -175.9(8)

C19a C14a C15a C16a . . . . 1.0(13)

C13a C14a C19a C18a . . . . 176.0(11)

C15a C14a C19a C18a . . . . -.3(17)

C14a C15a C16a N4a . . . . 177.5(9)

C14a C15a C16a C17a . . . . -1.0(13)

N4a C16a C17a N5a . . . . 2.6(11)

N4a C16a C17a C18a . . . . -178.3(10)

C15a C16a C17a N5a . . . . -178.8(10)

C15a C16a C17a C18a . . . . .3(16)

N5a C17a C18a C19a . . . . 179.6(9)

C16a C17a C18a C19a . . . . .5(14)

C17a C18a C19a C14a . . . . -.5(14)

N4a C20a C21a N6a . . . . 17.6(11)

N4a C20a C21a C22a . . . . -160.1(9)

N5a C20a C21a N6a . . . . -160.8(8)

N5a C20a C21a C22a . . . . 21.5(14)

N6a C21a C22a C23a . . . . 2.1(15)

C20a C21a C22a C23a . . . . 179.1(10)

C21a C22a C23a C24a . . . . 1.2(13)

C22a C23a C24a C25a . . . . -4.2(16)

C23a C24a C25a N6a . . . . 3.1(16)

C23a C24a C25a C26a . . . . -166.6(10)

N6a C25a C26a O1a . . . . -37.6(16)

N6a C25a C26a N7a . . . . 146.0(13)

C24a C25a C26a O1a . . . . 132.3(12)

C24a C25a C26a N7a . . . . -44.1(18)

C5b N1b C1b C2b . . . . 4.7(18)

C1b N1b C5b C4b . . . . -4.5(13)

C1b N1b C5b C6b . . . . -179.0(9)

C7b N2b C6b N3b . . . . -4.5(12)

C7b N2b C6b C5b . . . . 174.8(10)

C6b N2b C7b C8b . . . . -173.6(14)

C6b N2b C7b C12b . . . . 5.4(14)

C12b N3b C6b N2b . . . . 2.5(12)

C12b N3b C6b C5b . . . . -176.6(12)

C32b N3b C6b N2b . . . . -177.2(10)

C32b N3b C6b C5b . . . . 3.7(19)

C6b N3b C12b C7b . . . . .4(14)

C6b N3b C12b C11b . . . . 172.2(16)

C32b N3b C12b C7b . . . . -180.0(12)

C32b N3b C12b C11b . . . . -8(3)

C20b N4b C16b C15b . . . . 173.7(13)

C20b N4b C16b C17b . . . . -1.3(13)

C16b N4b C20b N5b . . . . 1.6(12)

C16b N4b C20b C21b . . . . -178.1(10)

C20b N5b C17b C16b . . . . .8(13)

C20b N5b C17b C18b . . . . -179.1(13)

C33b N5b C17b C16b . . . . -172.2(11)

C33b N5b C17b C18b . . . . 8(2)

C17b N5b C20b N4b . . . . -1.6(14)

C17b N5b C20b C21b . . . . 178.0(12)

C33b N5b C20b N4b . . . . 171.0(11)

C33b N5b C20b C21b . . . . -9(2)

C25b N6b C21b C20b . . . . -175.9(10)

C25b N6b C21b C22b . . . . 3.0(16)

C21b N6b C25b C24b . . . . -7.0(19)

C21b N6b C25b C26b . . . . 174.8(11)

C27b N7b C26b O1b . . . . -169.7(11)

C27b N7b C26b C25b . . . . 9.1(19)

C29b N7b C26b O1b . . . . 10.5(17)

C29b N7b C26b C25b . . . . -170.6(11)

C26b N7b C27b C28b . . . . 118.8(15)

C29b N7b C27b C28b . . . . -61.4(15)

C26b N7b C29b C30b . . . . -82.7(13)

C27b N7b C29b C30b . . . . 97.4(12)

N1b C1b C2b C3b . . . . -2.0(19)

N1b C1b C2b C31b . . . . 178.7(11)

C1b C2b C3b C4b . . . . .6(16)

C31b C2b C3b C4b . . . . 180.0(10)

C2b C3b C4b C5b . . . . -2(2)

C3b C4b C5b N1b . . . . 4.2(18)

C3b C4b C5b C6b . . . . 176.2(12)

N1b C5b C6b N2b . . . . -7.8(16)

N1b C5b C6b N3b . . . . 171.1(13)

C4b C5b C6b N2b . . . . -179.7(13)

C4b C5b C6b N3b . . . . 0(3)

N2b C7b C8b C9b . . . . 175.7(13)

C12b C7b C8b C9b . . . . -3.2(19)

N2b C7b C12b N3b . . . . -2.8(11)

N2b C7b C12b C11b . . . . -177.5(10)

C8b C7b C12b N3b . . . . 176.6(9)

C8b C7b C12b C11b . . . . 1.8(16)

C7b C8b C9b C10b . . . . 2.9(19)

C7b C8b C9b C13b . . . . -174.5(12)

C8b C9b C10b C11b . . . . -1.3(17)

C13b C9b C10b C11b . . . . 176.6(11)

C8b C9b C13b C14b . . . . -64.8(16)

C10b C9b C13b C14b . . . . 117.8(12)

C9b C10b C11b C12b . . . . 0(3)

C10b C11b C12b N3b . . . . -172.0(14)

C10b C11b C12b C7b . . . . 0(2)

C9b C13b C14b C15b . . . . -44.9(16)

C9b C13b C14b C19b . . . . 135.2(11)

C13b C14b C15b C16b . . . . -175.7(12)

C19b C14b C15b C16b . . . . 4.2(19)

C13b C14b C19b C18b . . . . 177.0(11)

C15b C14b C19b C18b . . . . -3.0(18)

C14b C15b C16b N4b . . . . -179.4(12)

C14b C15b C16b C17b . . . . -4.5(17)

N4b C16b C17b N5b . . . . .2(12)

N4b C16b C17b C18b . . . . -179.8(10)

C15b C16b C17b N5b . . . . -175.9(10)

C15b C16b C17b C18b . . . . 4.0(17)

N5b C17b C18b C19b . . . . 176.3(13)

C16b C17b C18b C19b . . . . -3.6(19)

C17b C18b C19b C14b . . . . 2.7(18)

N4b C20b C21b N6b . . . . -18.6(17)

N4b C20b C21b C22b . . . . 162.7(13)

N5b C20b C21b N6b . . . . 161.8(12)

N5b C20b C21b C22b . . . . -17(3)

N6b C21b C22b C23b . . . . 3.3(18)

C20b C21b C22b C23b . . . . -177.9(12)

C21b C22b C23b C24b . . . . -8(3)

C22b C23b C24b C25b . . . . 3.7(19)

C23b C24b C25b N6b . . . . 2.7(19)

C23b C24b C25b C26b . . . . -179.2(12)

N6b C25b C26b O1b . . . . 32.9(13)

N6b C25b C26b N7b . . . . -146.1(11)

C24b C25b C26b O1b . . . . -145.5(11)

C24b C25b C26b N7b . . . . 35.5(17)

C5c N1c C1c C2c . . . . 1.8(13)

C1c N1c C5c C4c . . . . -4.6(13)

C1c N1c C5c C6c . . . . 179.7(9)

C7c N2c C6c N3c . . . . -2.1(10)

C7c N2c C6c C5c . . . . 173.0(8)

C6c N2c C7c C8c . . . . -175.6(10)

C6c N2c C7c C12c . . . . 1.0(10)

C12c N3c C6c N2c . . . . 2.9(12)

C12c N3c C6c C5c . . . . -170.6(10)

C32c N3c C6c N2c . . . . -172.6(10)

C32c N3c C6c C5c . . . . 13.9(17)

C6c N3c C12c C7c . . . . -1.7(9)

C6c N3c C12c C11c . . . . 175.1(9)

C32c N3c C12c C7c . . . . 174.7(8)

C32c N3c C12c C11c . . . . -8.4(15)

C20c N4c C16c C15c . . . . 176.2(14)

C20c N4c C16c C17c . . . . -2.5(14)

C16c N4c C20c N5c . . . . 3.5(13)

C16c N4c C20c C21c . . . . -178.4(11)

C20c N5c C17c C16c . . . . 1.9(15)

C20c N5c C17c C18c . . . . -175.6(15)

C33c N5c C17c C16c . . . . -175.9(12)

C33c N5c C17c C18c . . . . 7(3)

C17c N5c C20c N4c . . . . -3.1(13)

C17c N5c C20c C21c . . . . 178.8(11)

C33c N5c C20c N4c . . . . 175.1(10)

C33c N5c C20c C21c . . . . -3.0(18)

C25c N6c C21c C20c . . . . -177.7(9)

C25c N6c C21c C22c . . . . 4.4(14)

C21c N6c C25c C24c . . . . -.7(17)

C21c N6c C25c C26c . . . . 172.5(10)

C27c N7c C26c O1c . . . . -4.5(16)

C27c N7c C26c C25c . . . . 176.8(10)

C29c N7c C26c O1c . . . . 169.1(11)

C29c N7c C26c C25c . . . . -9.7(17)

C26c N7c C27c C28c . . . . -93.4(13)

C29c N7c C27c C28c . . . . 92.2(13)

C26c N7c C29c C30c . . . . -70.5(13)

C27c N7c C29c C30c . . . . 102.3(12)

N1c C1c C2c C3c . . . . 1.8(14)

N1c C1c C2c C31c . . . . -176.4(9)

C1c C2c C3c C4c . . . . -3.5(16)

C31c C2c C3c C4c . . . . 174.4(11)

C2c C3c C4c C5c . . . . .8(15)

C3c C4c C5c N1c . . . . 2.8(12)

C3c C4c C5c C6c . . . . 178.4(9)

N1c C5c C6c N2c . . . . -2.1(11)

N1c C5c C6c N3c . . . . 171.9(8)

C4c C5c C6c N2c . . . . -177.8(8)

C4c C5c C6c N3c . . . . -3.8(15)

N2c C7c C8c C9c . . . . 175.2(9)

C12c C7c C8c C9c . . . . -1.5(12)

N2c C7c C12c N3c . . . . .7(11)

N2c C7c C12c C11c . . . . -176.0(10)

C8c C7c C12c N3c . . . . 177.5(9)

C8c C7c C12c C11c . . . . .8(15)

C7c C8c C9c C10c . . . . .1(15)

C7c C8c C9c C13c . . . . -173.7(9)

C8c C9c C10c C11c . . . . 2.8(17)

C13c C9c C10c C11c . . . . 176.7(11)

C8c C9c C13c C14c . . . . -31.9(12)

C10c C9c C13c C14c . . . . 153.2(9)

C9c C10c C11c C12c . . . . -3.0(14)

C10c C11c C12c N3c . . . . -173.9(11)

C10c C11c C12c C7c . . . . 1.9(16)

C9c C13c C14c C15c . . . . -61.3(16)

C9c C13c C14c C19c . . . . 122.6(12)

C13c C14c C15c C16c . . . . -175.8(11)

C19c C14c C15c C16c . . . . .6(18)

C13c C14c C19c C18c . . . . 178.0(11)

C15c C14c C19c C18c . . . . 1.1(17)

C14c C15c C16c N4c . . . . -179.6(13)

C14c C15c C16c C17c . . . . -1.0(19)

N4c C16c C17c N5c . . . . .4(12)

N4c C16c C17c C18c . . . . 178.7(10)

C15c C16c C17c N5c . . . . -178.7(10)

C15c C16c C17c C18c . . . . -.4(16)

N5c C17c C18c C19c . . . . 179.6(13)

C16c C17c C18c C19c . . . . 2.2(19)

C17c C18c C19c C14c . . . . -3(3)

N4c C20c C21c N6c . . . . -16.8(17)

N4c C20c C21c C22c . . . . 160.5(12)

N5c C20c C21c N6c . . . . 160.7(12)

N5c C20c C21c C22c . . . . -22(3)

N6c C21c C22c C23c . . . . -4.0(18)

C20c C21c C22c C23c . . . . 178.8(12)

C21c C22c C23c C24c . . . . -1.3(18)

C22c C23c C24c C25c . . . . 4.7(16)

C23c C24c C25c N6c . . . . -4.6(18)

C23c C24c C25c C26c . . . . -176.5(11)

N6c C25c C26c O1c . . . . -21.5(13)

N6c C25c C26c N7c . . . . 157.4(10)

C24c C25c C26c O1c . . . . 152.2(10)

C24c C25c C26c N7c . . . . -28.9(16)

O1d S1d C1d F1d . . . . -177.0(9)

O1d S1d C1d F2d . . . . 57.4(9)

O1d S1d C1d F3d . . . . -57.5(12)

O2d S1d C1d F1d . . . . -51.7(10)

O2d S1d C1d F2d . . . . -177.3(7)

O2d S1d C1d F3d . . . . 67.8(11)

O3d S1d C1d F1d . . . . 63.9(11)

O3d S1d C1d F2d . . . . -61.7(9)

O3d S1d C1d F3d . . . . -176.6(11)

O1e S1e C1e F1e . . . . 172.9(16)

O1e S1e C1e F2e . . . . -74.3(12)

O1e S1e C1e F3e . . . . 45(3)

O2e S1e C1e F1e . . . . 55.7(19)

O2e S1e C1e F2e . . . . 168.5(12)

O2e S1e C1e F3e . . . . -72(3)

O3e S1e C1e F1e . . . . -69(2)

O3e S1e C1e F2e . . . . 43.8(14)

O3e S1e C1e F3e . . . . 163(3)

O1f S1f C1f F1f . . . . -177.2(9)

O1f S1f C1f F2f . . . . -52.8(10)

O1f S1f C1f F3f . . . . 56.5(10)

O2f S1f C1f F1f . . . . 58.7(10)

O2f S1f C1f F2f . . . . -176.9(9)

O2f S1f C1f F3f . . . . -67.6(9)

O3f S1f C1f F1f . . . . -52.4(11)

O3f S1f C1f F2f . . . . 72.0(9)

O3f S1f C1f F3f . . . . -178.7(8)

O1g S1g C1g F1g . . . . -55.2(15)

O1g S1g C1g F2g . . . . 63.5(11)

O1g S1g C1g F3g . . . . -173.4(9)

O2g S1g C1g F1g . . . . -173.8(14)

O2g S1g C1g F2g . . . . -55.1(12)

O2g S1g C1g F3g . . . . 68.0(11)

O3g S1g C1g F1g . . . . 75.3(13)

O3g S1g C1g F2g . . . . -166.0(9)

O3g S1g C1g F3g . . . . -42.9(9)

O1g' S1g C1g' F1g' . . . . -52.6(15)

O1g' S1g C1g' F2g' . . . . -170.3(11)

O1g' S1g C1g' F3g' . . . . 64.6(14)

O2g' S1g C1g' F1g' . . . . -174.6(17)

O2g' S1g C1g' F2g' . . . . 67.6(17)

O2g' S1g C1g' F3g' . . . . -57.4(18)

O3g' S1g C1g' F1g' . . . . 61.7(16)

O3g' S1g C1g' F2g' . . . . -56.0(13)

O3g' S1g C1g' F3g' . . . . 178.9(14)

O1h S1h C1h F1h . . . . -176.8(12)

O1h S1h C1h F2h . . . . -57.3(13)

O1h S1h C1h F3h . . . . 64.3(12)

O2h S1h C1h F1h . . . . 68.2(12)

O2h S1h C1h F2h . . . . -172.3(10)

O2h S1h C1h F3h . . . . -50.7(11)

O3h S1h C1h F1h . . . . -55.6(12)

O3h S1h C1h F2h . . . . 63.9(12)

O3h S1h C1h F3h . . . . -174.5(10)

O1h' S1h' C1h' F1h' . . . . 69.7(15)

O1h' S1h' C1h' F2h' . . . . -49.2(12)

O1h' S1h' C1h' F3h' . . . . -172.0(10)

O2h' S1h' C1h' F1h' . . . . -55.0(15)

O2h' S1h' C1h' F2h' . . . . -174.0(10)

O2h' S1h' C1h' F3h' . . . . 63.3(11)

O3h' S1h' C1h' F1h' . . . . -173.9(15)

O3h' S1h' C1h' F2h' . . . . 67.1(13)

O3h' S1h' C1h' F3h' . . . . -55.6(13)

#=END===