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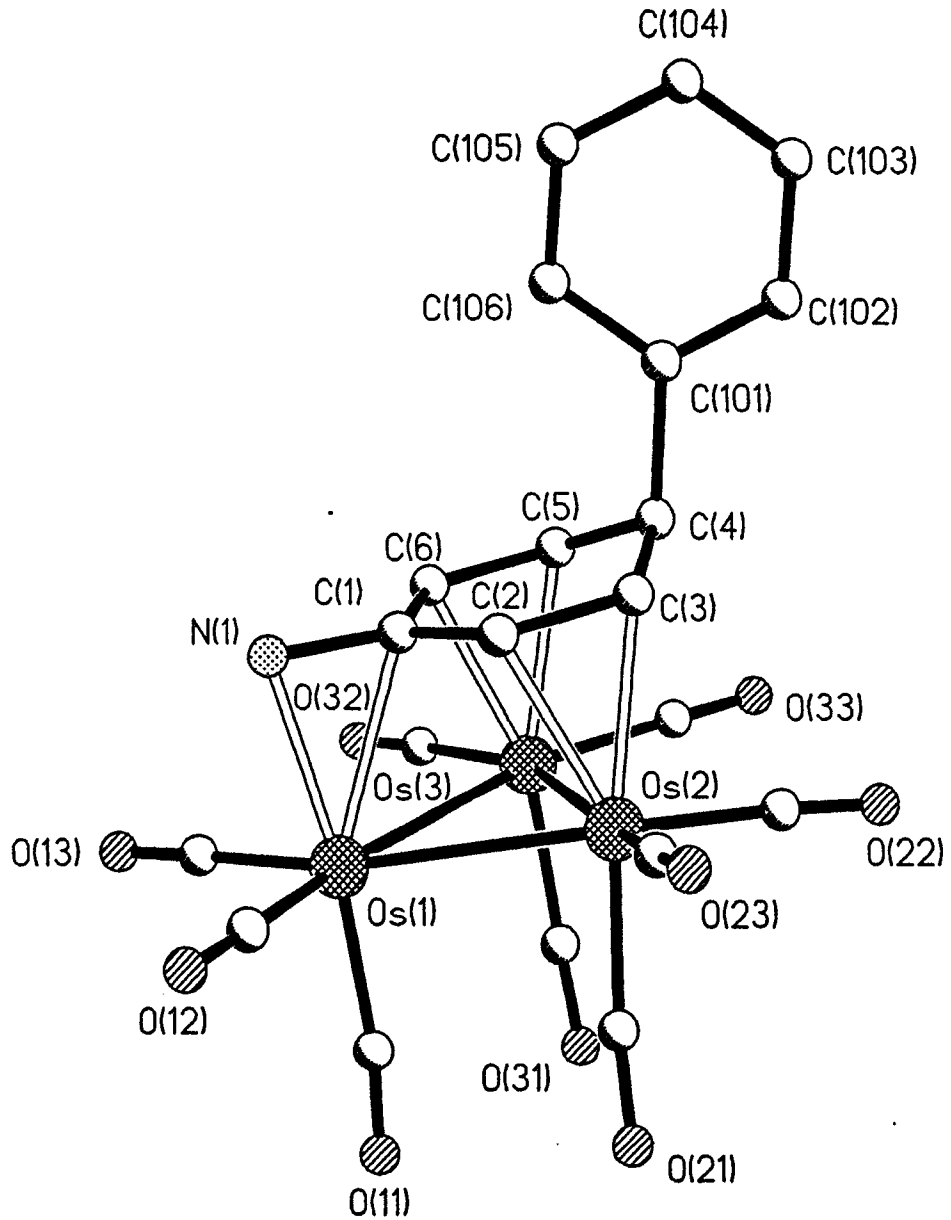
C(104)
C(105)
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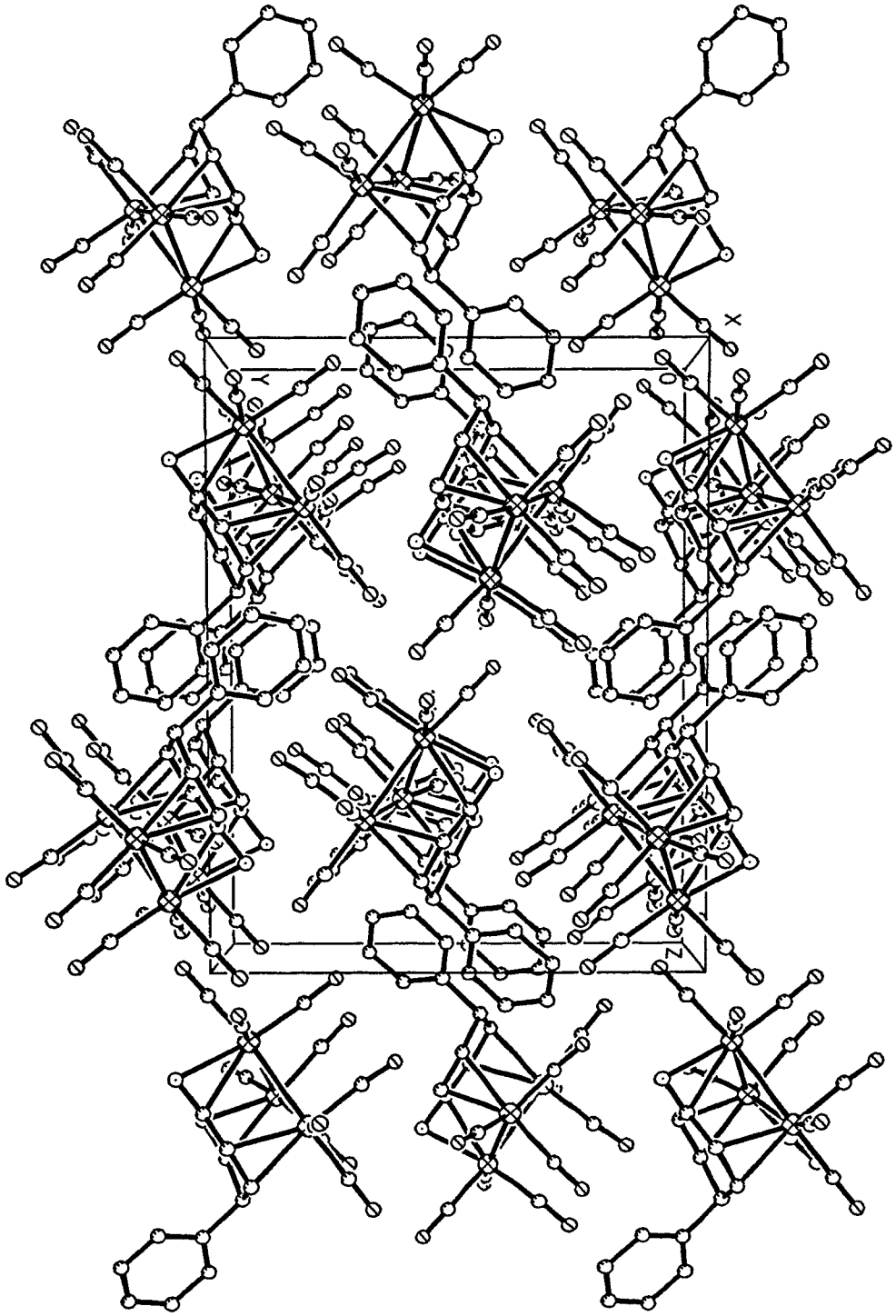
X
Y
Z

Table 1. Crystal data and structure refinement for 1.

Identification code	ljk02
Empirical formula	$C_{21}H_{11}NO_9Os_3$
Formula weight	991.91
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.199(10) Å α = 90° b = 13.332(11) Å β = 95.83(5)° c = 17.704(12) Å γ = 90°
Volume	2160(3) Å^3
Z	4
Density (calculated)	3.050 Mg/m^3
Absorption coefficient	17.659 mm^{-1}
F(000)	1776
Crystal size	0.30 x 0.25 x 0.25 mm
θ range for data collection	3.02 to 22.52°
Index ranges	$-9 \leq h \leq 9$, $-13 \leq k \leq 14$, $-18 \leq \ell \leq 19$
Reflections collected	3917
Independent reflections	2816 (R_{int} = 0.0349)
Absorption correction	Semi-empirical
Max. and min. transmission	0.329 and 0.143
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2814 / 0 / 197
Goodness-of-fit on F^2	1.180
Final R indices [$I>2\sigma(I)$]	R1 = 0.0358, wR2 = 0.0893
R indices (all data)	R1 = 0.0428, wR2 = 0.0975
Largest diff. peak and hole	2.686 and -1.512 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Os(1)	7845(1)	9333(1)	1249(1)	20(1)
Os(2)	5702(1)	8854(1)	2296(1)	16(1)
Os(3)	8638(1)	8100(1)	2576(1)	16(1)
N(1)	8567(13)	10797(8)	1820(6)	29(3)
C(1)	8155(14)	10271(9)	2416(7)	21(3)
C(2)	6719(14)	10359(9)	2630(7)	22(3)
C(3)	6304(14)	9891(9)	3304(6)	17(3)
C(4)	7509(13)	9501(9)	3894(6)	15(3)
C(5)	8877(14)	9262(9)	3563(6)	19(3)
C(6)	9274(16)	9725(10)	2897(7)	27(3)
C(101)	7748(13)	10326(9)	4504(6)	16(3)
C(102)	7068(15)	10241(10)	5154(7)	27(3)
C(103)	7174(16)	11014(10)	5685(8)	32(3)
C(104)	7905(16)	11858(10)	5563(7)	30(3)
C(105)	8625(17)	11953(11)	4919(8)	33(3)
C(106)	8552(15)	11189(9)	4397(7)	25(3)
C(11)	7261(16)	8209(11)	641(8)	31(3)
O(11)	7067(13)	7555(7)	239(5)	40(3)
C(12)	6789(15)	10220(10)	547(7)	27(3)
O(12)	6176(13)	10764(8)	119(6)	48(3)
C(13)	9693(17)	9385(10)	877(8)	30(3)
O(13)	10792(12)	9401(7)	640(5)	39(3)
C(21)	5030(15)	7930(10)	1512(7)	23(3)
O(21)	4549(11)	7349(8)	1086(5)	40(3)
C(22)	5340(14)	7925(9)	3064(7)	19(3)
O(22)	5082(11)	7334(7)	3506(5)	33(2)
C(23)	3907(16)	9573(10)	2111(7)	27(3)
O(23)	2820(12)	9988(8)	2034(6)	46(3)
C(31)	7950(15)	7006(10)	1944(7)	26(3)
O(31)	7615(14)	6310(7)	1595(6)	50(3)
C(32)	10634(15)	7893(9)	2413(6)	17(3)
O(32)	11786(11)	7763(7)	2289(6)	38(2)
C(33)	8599(14)	7272(9)	3454(7)	20(3)
O(33)	8605(11)	6759(6)	3960(5)	29(2)

Table 3. Bond lengths [Å] and angles [°] for 1.

Os(1)-C(13)	1.89(2)	Os(1)-C(11)	1.890(14)
Os(1)-C(12)	1.908(14)	Os(1)-N(1)	2.266(11)
Os(1)-C(1)	2.407(12)	Os(1)-Os(3)	2.900(2)
Os(1)-Os(2)	2.911(2)	Os(2)-C(22)	1.893(12)
Os(2)-C(23)	1.91(2)	Os(2)-C(21)	1.911(13)
Os(2)-C(2)	2.267(13)	Os(2)-C(3)	2.282(11)
Os(2)-Os(3)	2.877(3)	Os(3)-C(31)	1.906(14)
Os(3)-C(32)	1.907(14)	Os(3)-C(33)	1.910(13)
Os(3)-C(6)	2.301(13)	Os(3)-C(5)	2.330(12)
N(1)-C(1)	1.35(2)	C(1)-C(2)	1.42(2)
C(1)-C(6)	1.46(2)	C(2)-C(3)	1.43(2)
C(3)-C(4)	1.53(2)	C(4)-C(5)	1.48(2)
C(4)-C(101)	1.54(2)	C(5)-C(6)	1.41(2)
C(101)-C(102)	1.37(2)	C(101)-C(106)	1.39(2)
C(102)-C(103)	1.39(2)	C(103)-C(104)	1.34(2)
C(104)-C(105)	1.38(2)	C(105)-C(106)	1.37(2)
C(11)-O(11)	1.13(2)	C(12)-O(12)	1.15(2)
C(13)-O(13)	1.13(2)	C(21)-O(21)	1.14(2)
C(22)-O(22)	1.152(14)	C(23)-O(23)	1.14(2)
C(31)-O(31)	1.14(2)	C(32)-O(32)	1.12(2)
C(33)-O(33)	1.13(2)		

C(13)-Os(1)-C(11)	92.6(6)	C(13)-Os(1)-C(12)	99.7(6)
C(11)-Os(1)-C(12)	91.4(6)	C(13)-Os(1)-N(1)	83.7(5)
C(11)-Os(1)-N(1)	171.9(5)	C(12)-Os(1)-N(1)	82.1(5)
C(13)-Os(1)-C(1)	104.4(5)	C(11)-Os(1)-C(1)	154.4(5)
C(12)-Os(1)-C(1)	104.2(5)	N(1)-Os(1)-C(1)	33.5(4)
C(13)-Os(1)-Os(3)	98.2(4)	C(11)-Os(1)-Os(3)	92.6(4)
C(12)-Os(1)-Os(3)	161.5(4)	N(1)-Os(1)-Os(3)	95.1(3)
C(1)-Os(1)-Os(3)	66.5(3)	C(13)-Os(1)-Os(2)	157.4(4)
C(11)-Os(1)-Os(2)	90.9(4)	C(12)-Os(1)-Os(2)	102.5(4)
N(1)-Os(1)-Os(2)	95.3(3)	C(1)-Os(1)-Os(2)	66.2(3)
Os(3)-Os(1)-Os(2)	59.36(5)	C(22)-Os(2)-C(23)	103.8(5)
C(22)-Os(2)-C(21)	91.8(5)	C(23)-Os(2)-C(21)	89.4(6)
C(22)-Os(2)-C(2)	119.3(5)	C(23)-Os(2)-C(2)	85.8(5)
C(21)-Os(2)-C(2)	148.7(5)	C(22)-Os(2)-C(3)	83.2(5)
C(23)-Os(2)-C(3)	88.1(5)	C(21)-Os(2)-C(3)	173.7(5)
C(2)-Os(2)-C(3)	36.7(4)	C(22)-Os(2)-Os(3)	83.0(4)
C(23)-Os(2)-Os(3)	170.2(4)	C(21)-Os(2)-Os(3)	97.4(4)
C(2)-Os(2)-Os(3)	84.8(3)	C(3)-Os(2)-Os(3)	85.9(3)
C(22)-Os(2)-Os(1)	141.3(4)	C(23)-Os(2)-Os(1)	114.2(4)
C(21)-Os(2)-Os(1)	82.5(4)	C(2)-Os(2)-Os(1)	71.6(3)
C(3)-Os(2)-Os(1)	103.8(3)	Os(3)-Os(2)-Os(1)	60.12(6)
C(31)-Os(3)-C(32)	93.9(5)	C(31)-Os(3)-C(33)	90.2(5)
C(32)-Os(3)-C(33)	97.9(5)	C(31)-Os(3)-C(6)	157.9(5)
C(32)-Os(3)-C(6)	87.1(5)	C(33)-Os(3)-C(6)	111.6(5)
C(31)-Os(3)-C(5)	161.7(5)	C(32)-Os(3)-C(5)	101.0(5)
C(33)-Os(3)-C(5)	77.4(5)	C(6)-Os(3)-C(5)	35.5(4)
C(31)-Os(3)-Os(2)	85.2(4)	C(32)-Os(3)-Os(2)	157.8(3)
C(33)-Os(3)-Os(2)	104.3(4)	C(6)-Os(3)-Os(2)	85.7(4)
C(5)-Os(3)-Os(2)	85.0(3)	C(31)-Os(3)-Os(1)	85.2(4)
C(32)-Os(3)-Os(1)	97.3(3)	C(33)-Os(3)-Os(1)	164.4(4)
C(6)-Os(3)-Os(1)	72.7(3)	C(5)-Os(3)-Os(1)	103.2(3)
Os(2)-Os(3)-Os(1)	60.52(4)	C(1)-N(1)-Os(1)	79.0(7)
N(1)-C(1)-C(2)	120.6(12)	N(1)-C(1)-C(6)	118.4(12)
C(2)-C(1)-C(6)	120.4(11)	N(1)-C(1)-Os(1)	67.5(7)
C(2)-C(1)-Os(1)	104.0(8)	C(6)-C(1)-Os(1)	104.9(8)
C(1)-C(2)-C(3)	121.5(12)	C(1)-C(2)-Os(2)	103.2(8)
C(3)-C(2)-Os(2)	72.2(7)	C(2)-C(3)-C(4)	118.6(11)

C(2)-C(3)-Os(2)	71.1(7)	C(4)-C(3)-Os(2)	115.4(7)
C(5)-C(4)-C(3)	112.9(10)	C(5)-C(4)-C(101)	111.4(10)
C(3)-C(4)-C(101)	106.1(9)	C(6)-C(5)-C(4)	122.7(12)
C(6)-C(5)-Os(3)	71.1(7)	C(4)-C(5)-Os(3)	115.0(8)
C(5)-C(6)-C(1)	118.5(12)	C(5)-C(6)-Os(3)	73.4(7)
C(1)-C(6)-Os(3)	100.3(8)	C(102)-C(101)-C(106)	118.6(11)
C(102)-C(101)-C(4)	119.0(11)	C(106)-C(101)-C(4)	122.3(10)
C(101)-C(102)-C(103)	120.0(13)	C(104)-C(103)-C(102)	121.0(13)
C(103)-C(104)-C(105)	120.0(13)	C(106)-C(105)-C(104)	119.5(14)
C(105)-C(106)-C(101)	120.8(13)	O(11)-C(11)-Os(1)	171.5(13)
O(12)-C(12)-Os(1)	178.6(12)	O(13)-C(13)-Os(1)	178.4(13)
O(21)-C(21)-Os(2)	174.2(12)	O(22)-C(22)-Os(2)	176.9(11)
O(23)-C(23)-Os(2)	176.7(12)	O(31)-C(31)-Os(3)	175.0(12)
O(32)-C(32)-Os(3)	177.2(11)	O(33)-C(33)-Os(3)	177.5(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Os(1)	29(1)	15(1)	16(1)	1(1)	5(1)	-5(1)
Os(2)	18(1)	13(1)	18(1)	0(1)	-1(1)	-2(1)
Os(3)	19(1)	12(1)	18(1)	-1(1)	3(1)	2(1)
O(11)	72(8)	27(6)	24(5)	-11(4)	12(5)	-24(5)
O(12)	53(8)	46(7)	43(6)	19(5)	-3(5)	2(6)
O(13)	42(7)	36(6)	41(6)	4(5)	13(5)	-2(5)
O(21)	42(7)	39(6)	39(6)	-14(5)	3(5)	-18(5)
O(22)	35(6)	27(5)	38(5)	7(4)	14(4)	-5(5)
O(23)	34(7)	38(6)	61(7)	-4(5)	-16(5)	15(5)
O(31)	83(9)	22(5)	41(6)	-11(5)	-4(6)	-5(6)
O(32)	31(6)	33(6)	51(6)	1(5)	16(5)	-1(5)
O(33)	41(6)	24(5)	25(5)	1(4)	11(4)	-1(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	6014(14)	10736(9)	2320(7)	26
H(3A)	5303(14)	9823(9)	3385(6)	20
H(4A)	7150(13)	8882(9)	4134(6)	19
H(5A)	9517(14)	8777(9)	3809(6)	22
H(6A)	10247(16)	9683(10)	2764(7)	33
H(10A)	6524(15)	9655(10)	5242(7)	32
H(10B)	6722(16)	10942(10)	6141(8)	38
H(10C)	7928(16)	12392(10)	5920(7)	36
H(10D)	9167(17)	12543(11)	4837(8)	40
H(10E)	9058(15)	11250(9)	3957(7)	31