of RS = 0.092 Å towards the C(2) atom are found. The corresponding values for the hinge angle and fold angle are HA = 4.8° and FA = 5.4°. The differences in the bond lengths in the five membered ring are 0.06 Å.

As discussed for the rhodium structures the values are in the expected range for distorted η^5-coordination, too. But **14a** shows a significant weaker tendency towards a $\eta^2+\eta^3$-coordination than the analogous rhodium complex **7a**, as besides possible packing effects the stronger back bonding of iridium to the neutral ligand increases the lewis acidity of the metal and therefore the η^5-coordination is favored. The diene systems of the COD ligand are again aligned parallel to the longitudinal axis of indene due to the orbital control. In these cases the rotation angle of 19.0° is in close accordance to the value of the rhodium complexes and bigger than the theoretical value as well. The structure parameters are compiled in Table ??.

Table 1. Crystal data and structure refinement for **14a**.

Identification code	14a	
Empirical formula	$C_{29}H_{41}Ir$	
Formula weight	581.82	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$ (No.19)	
Unit cell dimensions	a = 9.1902(1) Å	α= 90°.
	b = 12.6546(2) Å	β= 90°.
	c = 20.9402(2) Å	γ= 90°.
Volume	2435.31(5) $Å^3$	
Z	4	
Density (calculated)	1.587 g/cm^3	
Absorption coefficient	5.496 mm^{-1}	
F(000)	1168	
Crystal size	0.38 x 0.44 x 0.44 mm^3	
Theta range for data collection	1.88 to 27.50°.	
Index ranges	-11<=h<=11, -15<=k<=16, -27<=l<=27	
Reflections collected	18928	
Independent reflections	5567 [R(int) = 0.0373]	
Completeness to theta = 27.50°	99.7 %	
Absortion correction	SADABS (max/min trans.: 0.252462 / 0.158880)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5567 / 0 / 276	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0505	
R indices (all data)	R1 = 0.0239, wR2 = 0.0510	
Absolute structure parameter	-0.005(8)	
Largest diff. peak and hole	0.939 and -1.464 e/$Å^3$	

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **14a**. U(eq) is defined as one third of the trace of the orthogonalized U(ij) tensor.

Atom	x	y	z	U(eq)
Ir	3680(1)	3442(1)	2978(1)	17(1)
C(1)	5340(4)	4175(3)	3625(2)	17(1)
C(2)	5093(4)	4883(3)	3100(2)	20(1)
C(3)	5496(4)	4383(3)	2526(2)	23(1)
C(4)	6128(4)	3379(3)	2673(2)	22(1)
C(5)	6790(5)	2611(4)	2265(2)	30(1)
C(6)	7323(4)	1724(4)	2556(2)	36(1)
C(7)	7153(4)	1529(4)	3222(2)	32(1)
C(8)	6512(4)	2253(3)	3626(2)	23(1)
C(9)	6033(4)	3229(3)	3356(2)	18(1)
C(10)	6885(6)	2807(5)	1563(2)	48(2)
C(11)	6240(6)	1963(3)	4316(2)	35(1)
C(12)	5328(4)	4562(3)	4307(2)	19(1)
C(13)	3841(4)	5025(3)	4500(2)	22(1)
C(14)	3803(5)	5537(3)	5167(2)	24(1)
C(15)	5034(4)	6328(4)	5241(2)	28(1)
C(16)	6496(4)	5830(3)	5089(2)	26(1)
C(17)	6529(4)	5415(3)	4399(2)	19(1)
C(18)	2311(5)	6059(4)	5279(2)	32(1)
C(19)	8062(4)	5058(3)	4180(2)	23(1)
C(20)	9054(4)	6003(3)	4066(2)	29(1)
C(21)	8781(6)	4304(4)	4651(2)	40(1)
C(22)	1615(4)	3643(4)	3399(2)	26(1)
C(23)	2259(5)	2691(4)	3628(2)	29(1)
C(24)	1803(5)	1599(5)	3414(3)	43(1)
C(25)	1716(5)	1517(4)	2688(2)	38(1)
C(26)	2760(4)	2273(4)	2368(2)	31(1)
C(27)	2356(4)	3291(4)	2154(2)	29(1)

Table 2. (cont.)

C(28)	831(5)	3737(4)	2242(2)	35(1)
C(29)	332(4)	3667(4)	2935(2)	31(1)

Table 3. Bond lengths [Å] for **14a**.

Atoms	Bond length
Ir-Cg	1.9272(17)
Ir-C(1)	2.241(4)
Ir-C(2)	2.253(4)
Ir-C(3)	2.257(4)
Ir-C(4)	2.339(3)
Ir-C(9)	2.319(4)
Ir-C(22)	2.108(4)
Ir-C(23)	2.112(4)
Ir-C(26)	2.130(4)
Ir-C(27)	2.119(4)
C(1)-C(2)	1.436(5)
C(2)-C(3)	1.409(6)
C(3)-C(4)	1.431(6)
C(4)-C(5)	1.431(6)
C(5)-C(6)	1.368(7)
C(6)-C(7)	1.425(7)
C(7)-C(8)	1.379(6)
C(8)-C(9)	1.429(5)
C(9)-C(1)	1.468(5)
C(9)-C(4)	1.444(5)
C(5)-C(10)	1.493(7)

Atoms	Bond length
C(8)-C(11)	1.511(6)
C(1)-C(12)	1.511(5)
C(12)-C(13)	1.541(5)
C(13)-C(14)	1.540(5)
C(14)-C(15)	1.519(6)
C(15)-C(16)	1.518(6)
C(16)-C(17)	1.537(5)
C(17)-C(12)	1.555(5)
C(14)-C(18)	1.540(6)
C(17)-C(19)	1.550(5)
C(19)-C(20)	1.523(6)
C(19)-C(21)	1.523(6)
C(22)-C(23)	1.425(6)
C(23)-C(24)	1.512(7)
C(24)-C(25)	1.527(7)
C(25)-C(26)	1.512(7)
C(26)-C(27)	1.413(7)
C(27)-C(28)	1.521(6)
C(28)-C(29)	1.525(7)
C(29)-C(22)	1.528(5)

Cg = C(1), C(2), C(3), C(4), C(9)

Cg Ring-Slippage: 0.092 Å

SD: Δ = d {(Ir-C(4,9))-(Ir-C(1,3))} = 2.329 - 2.249 = 0.080 Å

HA: (C1,C2,C3)-(C1,C9,C4,C3) = 4.76 (0.44)

FA: (C1,C2,C3)-(C4,C5,C6,C7,C8,C9) = 5.43 (0.41)

Table 4. Bond angles [°] for **14a**.

Atoms	Bond angle
C(22)-Ir-Cg	138.71(13)
C(23)-Ir-Cg	133.15(13)
C(26)-Ir-Cg	132.61(11)
C(27)-Ir-Cg	129.33(12)
C(22)-Ir-C(23)	39.46(18)
C(26)-Ir-C(27)	38.86(19)
C(22)-Ir-C(27)	80.48(15)
C(23)-Ir-C(26)	80.11(18)
C(22)-Ir-C(26)	88.70(16)
C(23)-Ir-C(27)	97.39(17)
C(22)-C(23)-Ir	70.1(2)
C(23)-C(22)-Ir	70.4(2)
C(29)-C(22)-Ir	115.5(3)
C(24)-C(23)-Ir	113.1(3)
C(25)-C(26)-Ir	115.2(3)
C(28)-C(27)-Ir	113.4(3)
C(26)-C(27)-Ir	71.0(2)
C(27)-C(26)-Ir	70.2(2)
C(2)-C(1)-C(9)	106.5(3)
C(2)-C(1)-C(12)	121.3(3)
C(9)-C(1)-C(12)	129.1(3)
C(3)-C(2)-C(1)	109.3(4)
C(2)-C(3)-C(4)	108.8(3)
C(5)-C(4)-C(3)	130.3(4)
C(5)-C(4)-C(9)	121.9(4)
C(3)-C(4)-C(9)	107.8(3)
C(6)-C(5)-C(4)	116.3(4)
C(6)-C(5)-C(10)	123.6(4)
C(4)-C(5)-C(10)	120.1(5)
C(5)-C(6)-C(7)	122.5(4)

Atoms	Bond angle
C(8)-C(7)-C(6)	122.2(5)
C(7)-C(8)-C(9)	117.5(4)
C(7)-C(8)-C(11)	119.8(4)
C(9)-C(8)-C(11)	122.5(4)
C(8)-C(9)-C(4)	119.1(4)
C(8)-C(9)-C(1)	133.3(4)
C(4)-C(9)-C(1)	107.4(3)
C(1)-C(12)-C(13)	112.2(3)
C(1)-C(12)-C(17)	109.7(3)
C(13)-C(12)-C(17)	109.4(3)
C(14)-C(13)-C(12)	114.7(3)
C(15)-C(14)-C(13)	110.6(3)
C(15)-C(14)-C(18)	111.4(3)
C(13)-C(14)-C(18)	109.8(3)
C(16)-C(15)-C(14)	111.3(4)
C(15)-C(16)-C(17)	110.9(3)
C(16)-C(17)-C(19)	113.3(3)
C(16)-C(17)-C(12)	109.8(3)
C(19)-C(17)-C(12)	113.9(3)
C(20)-C(19)-C(21)	109.5(4)
C(20)-C(19)-C(17)	111.2(3)
C(21)-C(19)-C(17)	112.7(4)
C(23)-C(22)-C(29)	123.4(4)
C(22)-C(23)-C(24)	123.9(4)
C(23)-C(24)-C(25)	111.8(5)
C(26)-C(25)-C(24)	111.4(4)
C(27)-C(26)-C(25)	123.4(4)
C(26)-C(27)-C(28)	122.8(4)
C(27)-C(28)-C(29)	111.7(4)
C(28)-C(29)-C(22)	112.0(3)

Table 5. Anisotropic displacement parameters ($Å^2x10^3$)for **14a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U(11) + ... + 2 h k a^* b^* U(12)]$

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Ir	13(1)	19(1)	18(1)	-3(1)	0(1)	-2(1)
C(1)	15(2)	15(2)	21(2)	2(1)	0(1)	-1(1)
C(2)	21(2)	20(2)	20(2)	1(1)	-3(1)	-3(1)
C(3)	23(2)	27(2)	19(2)	2(2)	2(2)	-7(2)
C(4)	13(2)	27(2)	25(2)	-9(2)	3(1)	-4(2)
C(5)	18(2)	41(3)	31(2)	-15(2)	9(2)	-7(2)
C(6)	19(2)	35(3)	55(3)	-28(2)	3(2)	-2(2)
C(7)	20(2)	22(2)	53(3)	-9(2)	1(2)	3(2)
C(8)	16(2)	17(2)	38(2)	-3(2)	-4(2)	-1(2)
C(9)	14(2)	17(2)	23(2)	-5(1)	1(1)	-3(1)
C(10)	40(3)	74(4)	30(3)	-25(3)	8(2)	-12(3)
C(11)	37(2)	21(2)	47(3)	9(2)	1(2)	3(2)
C(12)	19(2)	19(2)	18(2)	0(1)	-2(1)	2(2)
C(13)	18(2)	25(2)	22(2)	-4(1)	1(2)	2(2)
C(14)	27(2)	26(2)	19(2)	-3(1)	1(2)	0(2)
C(15)	28(2)	31(3)	25(2)	-11(2)	0(2)	1(2)
C(16)	23(2)	30(2)	25(2)	-8(2)	-5(2)	-2(2)
C(17)	16(2)	21(2)	22(2)	-5(1)	-1(1)	-2(2)
C(18)	29(2)	39(3)	27(2)	-5(2)	6(2)	6(2)
C(19)	18(2)	24(2)	27(2)	-7(2)	-1(2)	1(2)
C(20)	19(2)	30(2)	39(2)	2(2)	1(2)	-3(2)
C(21)	23(2)	32(2)	66(3)	9(2)	-1(2)	10(2)
C(22)	11(2)	35(3)	30(2)	-11(2)	4(1)	-3(2)
C(23)	21(2)	38(3)	27(2)	3(2)	0(2)	-10(2)
C(24)	33(2)	33(3)	64(3)	10(3)	-2(2)	-13(2)
C(25)	26(2)	26(2)	62(3)	-14(2)	-3(2)	-4(2)
C(26)	17(2)	40(3)	36(2)	-22(2)	0(2)	-6(2)
C(27)	20(2)	46(3)	22(2)	-9(2)	-2(1)	-7(2)

Table 5. (cont.)

C(28)	23(2)	46(3)	37(2)	-2(2)	-10(2)	-3(2)
C(29)	19(2)	37(2)	36(2)	-11(2)	-1(2)	1(2)

Table 6. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **14a**.

Atom	x	y	z	U(eq)	bonded to
H(2)	4726	5565	3134	80	C(2)
H(3)	5372	4659	2118	80	C(3)
H(6)	7816	1228	2309	80	C(6)
H(7)	7485	893	3390	80	C(7)
H(10A)	7463	2265	1367	80	C(10)
H(10B)	7327	3483	1488	80	
H(10C)	5925	2800	1382	80	
H(11A)	6425	1223	4376	80	C(11)
H(11B)	5247	2116	4424	80	
H(11C)	6877	2367	4586	80	
H(12)	5546	3964	4589	80	C(12)
H(13A)	3561	5552	4187	80	C(13)
H(13B)	3122	4465	4487	80	
H(14)	3933	4979	5487	80	C(14)
H(15A)	4869	6922	4958	80	C(15)
H(15B)	5046	6593	5676	80	
H(16A)	6678	5252	5382	80	C(16)
H(16B)	7260	6350	5146	80	
H(17)	6258	6012	4125	80	C(17)
H(18A)	2320	6426	5680	80	C(18)
H(18B)	1568	5526	5286	80	
H(18C)	2115	6551	4941	80	
H(19)	7952	4684	3773	80	C(19)
H(20A)	9202	6373	4461	80	C(20)
H(20B)	8612	6469	3761	80	
H(20C)	9974	5762	3905	80	

Table 6. (cont.)

H(21A)	9644	4012	4462	80	C(21)
H(21B)	8118	3743	4754	80	
H(21C)	9034	4681	5033	80	
H(22)	1995	4283	3540	80	C(22)
H(23)	3005	2745	3926	80	C(23)
H(24A)	860	1433	3596	80	C(24)
H(24B)	2497	1084	3573	80	
H(25A)	1944	800	2558	80	C(25)
H(25B)	731	1673	2550	80	
H(26)	3718	2058	2308	80	C(26)
H(27)	3051	3707	1952	80	C(27)
H(28A)	158	3348	1973	80	C(28)
H(28B)	819	4470	2106	80	
H(29A)	-247	3033	2992	80	C(29)
H(29B)	-280	4270	3033	80	