$Ir_4(CO)_{12}$

Structure Types

$Ir[CO]_3$	*hP*116	(143) $P3 - d^{37}cb^2a^2$

$Ir_4(CO)_{12}$ [1]
Structural features: $Ir_4(CO)_{12}$ molecules consisting of a Ir_4 tetrahedral cluster with three CO units bonded to each Ir (partial orientational disorder).
Churchill M.R., Hutchinson J.P. (1978) [1]
C_3IrO_3
a = 1.32902, c = 0.89809 nm, c/a = 0.676, V = 1.3738 nm^3, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	3*d*	1	0.014	0.4398	0.8341		single atom C
C2	3*d*	1	0.0249	0.1391	0.9141	0.833	
Ir3	3*d*	1	0.0354	0.1327	0.0832	0.167	single atom C
C4	3*d*	1	0.0377	0.1789	0.971	0.167	
O5	3*d*	1	0.04	0.2237	0.8618		
O6	3*d*	1	0.0837	0.3256	0.5081		
C7	3*d*	1	0.1038	0.0823	0.4615	0.167	
C8	3*d*	1	0.128	0.4212	0.4753	0.555	
Ir9	3*d*	1	0.1304	0.0948	0.243	0.833	non-colinear CIr
C10	3*d*	1	0.1446	0.2591	0.1235	0.167	
C11	3*d*	1	0.1554	0.12	0.4236	0.833	
O12	3*d*	1	0.1576	0.5523	0.0842		
C13	3*d*	1	0.168	0.4094	0.534	0.445	
O14	3*d*	1	0.1725	0.1368	0.5479		non-colinear C_2
C15	3*d*	1	0.1741	0.5629	0.2094	0.555	
C16	3*d*	1	0.1876	0.2539	0.1857	0.833	
Ir17	3*d*	1	0.2019	0.5809	0.4205	0.555	single atom Ir
O18	3*d*	1	0.2215	0.3481	0.1518		
C19	3*d*	1	0.2233	0.595	0.1781	0.445	
C20	3*d*	1	0.2405	0.0261	0.1197	0.167	
C21	3*d*	1	0.2607	0.0777	0.1809	0.833	
O22	3*d*	1	0.2627	0.441	0.8386		
C23	3*d*	1	0.2749	0.4803	0.7226	0.445	
C24	3*d*	1	0.289	0.5251	0.7756	0.555	
Ir25	3*d*	1	0.2907	0.5315	0.5717	0.445	single atom C
O26	3*d*	1	0.3284	0.2701	0.8419		single atom C
O27	3*d*	1	0.3374	0.0677	0.1444		
C28	3*d*	1	0.3373	0.4378	0.5315	0.445	
O29	3*d*	1	0.3688	0.3743	0.5043		
C30	3*d*	1	0.3873	0.4652	0.4734	0.555	
C31	3*d*	1	0.4049	0.2584	0.81		single atom O
C32	3*d*	1	0.4678	0.082	0.8041		single atom O
O33	3*d*	1	0.493	0.228	0.4111		single atom C

(*continued*)

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site	Wyck.	sym.	x	y	z	occ.	atomic environment
C34	3*d*	1	0.5086	0.2318	0.5363		single atom O
Ir35	3*d*	1	0.5362	0.2385	0.7553		non-coplanar triangle C_3
O36	3*d*	1	0.5958	0.102	0.2051		single atom C
C37	3*d*	1	0.6204	0.1822	0.1342		single atom O
Ir38	1*c*	3..	$^2/_3$	$^1/_3$	0.0007		non-coplanar triangle C_3
Ir39	1*b*	3..	$^1/_3$	$^2/_3$	0.3355	0.445	trigonal prism Ir_3C_3
Ir40	1*b*	3..	$^1/_3$	$^2/_3$	0.6697	0.555	trigonal prism Ir_3C_3
Ir41	1*a*	3..	0	0	0.0	0.833	trigonal prism Ir_3C_3
Ir42	1*a*	3..	0	0	0.3311	0.167	trigonal prism C_3Ir_3

Transformation from published data: *y*,*x*,*z*
Experimental: single crystal, diffractometer, X-rays, wR = 0.047
Remarks: Short interatomic distances for partly occupied site(s).

References

[1] Churchill M.R., Hutchinson J.P. (1978), Inorg. Chem. 17, 3528–3535.

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