

$\text{ReOs}_3\text{H}_5[\text{CO}]_{12}$ $hP168$ $(176) P6_3/m - i^{11}h^6$ **($\mu\text{-H}$) $_5\text{Os}_3\text{Re}(\text{CO})_{12}$ [1]**

Structural features: $\text{ReH}_5\text{Os}_3(\text{CO})_{12}$ tetrahedral units (a (ReOs_3) tetrahedron with three $\text{C}=\text{O}$ units bonded to each vertex; probably one H above each Os-Os edge and above two of the Re-Os edges in statistical disorder with respect to a mirror plane).

Churchill M.R. et al. (1988) [1]

 $\text{C}_{12}\text{O}_{12}\text{Os}_3\text{Re}$ $a = 1.9087$, $c = 1.0963$ nm, $c/a = 0.574$, $V = 3.4589$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Os1	12i	1	0.0493	0.32905	0.1148		non-coplanar triangle C_3
C2	12i	1	0.0557	0.2455	0.0344		single atom O
C3	12i	1	0.0718	0.5324	0.1293		single atom O
O4	12i	1	0.0806	0.5746	0.0482		single atom C
O5	12i	1	0.1969	0.1344	0.0156		single atom C
C6	12i	1	0.2628	0.5154	0.1263		single atom O
O7	12i	1	0.301	0.5604	0.0485		single atom C
C8	12i	1	0.3488	0.0637	0.0965		single atom O
O9	12i	1	0.3875	0.1347	0.0906		single atom C
C10	12i	1	0.3957	0.3213	0.0219		single atom O
O11	12i	1	0.4415	0.345	0.1048		single atom C
Os12	6h	$m..$	0.05362	0.45785	$\frac{1}{4}$		non-coplanar triangle C_3
Re13	6h	$m..$	0.20221	0.44303	$\frac{1}{4}$		non-coplanar triangle C_3
C14	6h	$m..$	0.2698	0.3965	$\frac{1}{4}$		single atom O
O15	6h	$m..$	0.3066	0.3662	$\frac{1}{4}$		single atom C
C16	6h	$m..$	0.4705	0.0598	$\frac{1}{4}$		single atom O
O17	6h	$m..$	0.5177	0.1278	$\frac{1}{4}$		single atom C

Transformation from published data: $y, x, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.054$, $T = 297$ K

Remarks: H not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Churchill M.R., Fetting J.C., Hollander F.J., Lashewycz R.A. (1988), J. Organomet. Chem. 340, 367-376.