| $Ca_{4.74}Ir_3O_{12}$ | *hP*20 | (189) *P*-62*m* – kgf$^3$c |
|---|---|---|

**$Ca_{5-x}Ir_3O_{12}$** [1]; $K_5Dy_3I_{12}$ [2]
Structural features: Infinite chains of edge-linked $IrO_6$ octahedra. Vacancy derivative of $Ca_2IrO_4$ ($V_4P_2C$ antitype).

Dijksma F.J.J. et al. (1993) [1]
$Ca_{4.74}Ir_3O_{12}$
$a$ = 0.94235, $c$ = 0.31945 nm, $c/a$ = 0.339, $V$ = 0.2457 nm$^3$, $Z$ = 1

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 6*k* | *m*.. | 0.2381 | 0.4407 | $^1/_2$ | | single atom Ir |
| Ir2 | 3*g* | *m*2*m* | 0.33 | 0 | $^1/_2$ | | octahedron $O_6$ |
| O3 | 3*f* | *m*2*m* | 0.1958 | 0 | 0 | | non-colinear $Ir_2$ |
| O4 | 3*f* | *m*2*m* | 0.4602 | 0 | 0 | | non-colinear $Ir_2$ |
| Ca5 | 3*f* | *m*2*m* | 0.7123 | 0 | 0 | 0.912 | monocapped trigonal prism $O_7$ |
| Ca6 | 2*c* | -6.. | $^1/_3$ | $^2/_3$ | 0 | | tricapped trigonal prism $O_9$ |

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p$ = 0.027, T = 295 K

References: [1] Dijksma F.J.J., Vente J.F., Frikkee E., Ijdo D.J.W. (1993), Mater. Res. Bull. 28, 1145-1151. [2] Schilling G., Böcker M., Möller A., Meyer G. (2001), Z. Anorg. Allg. Chem. 627, 1309-1312.