| $Cs_{8.36}Mo_{12}[MoO_4][PO_4]_{10}O_{18}[H_2O]$ | *hP*214 | (176) $P6_3/m$ – $i^{10}h^{12}f^4eb$ |
|---|---|---|

**$Cs_{8+x}(MoO_4)Mo_{12}(PO_4)_{10}O_{18}\cdot H_2O$** [1]
Structural features: Units of four edge- and vertex-linked $MoO_6$ octahedra share vertices with $MoO_4$ and $PO_4$ tetrahedra (in part orientational disorder up-down) to form a 3D-framework; Cs and $H_2O$ in large channels parallel to [001].

Hoareau T. et al. (1994) [1]
$Cs_{8.35}H_2Mo_{13}O_{63}P_{10}$
$a$ = 1.6678, $c$ = 1.2717 nm, $c/a$ = 0.763, $V$ = 3.0634 nm$^3$, $Z$ = 2

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*i* | 1 | 0.0352 | 0.3006 | 0.022 | | single atom P |
| Cs2 | 12*i* | 1 | 0.13674 | 0.61455 | 0.0517 | | trigonal bipyramid $O_5$ |
| Cs3 | 12*i* | 1 | 0.1394 | 0.1862 | 0.152 | 0.152 | |
| O4 | 12*i* | 1 | 0.1664 | 0.4501 | 0.092 | | single atom P |
| O5 | 12*i* | 1 | 0.1907 | 0.0468 | 0.136 | | single atom Mo |
| Mo6 | 12*i* | 1 | 0.29419 | 0.05637 | 0.1452 | | pentagonal bipyramid $O_6Mo$ |
| O7 | 12*i* | 1 | 0.3511 | 0.1524 | 0.025 | | single atom P |
| P8 | 12*i* | 1 | 0.3827 | 0.2519 | 0.0013 | | tetrahedron $O_4$ |
| O9 | 12*i* | 1 | 0.4273 | 0.0645 | 0.152 | | single atom P |
| O10 | 12*i* | 1 | 0.441 | 0.313 | 0.092 | | single atom P |
| O11 | 6*h* | *m*.. | 0.049 | 0.309 | $^1/_4$ | | non-coplanar triangle $Mo_3$ |
| O12 | 6*h* | *m*.. | 0.074 | 0.487 | $^1/_4$ | | single atom P |
| Cs13 | 6*h* | *m*.. | 0.141 | 0.1829 | $^1/_4$ | 0.214 | |
| Mo14 | 6*h* | *m*.. | 0.1693 | 0.4384 | $^1/_4$ | | octahedron $O_6$ |
| O15 | 6*h* | *m*.. | 0.237 | 0.392 | $^1/_4$ | | single atom Mo |
| O16 | 6*h* | *m*.. | 0.265 | 0.57 | $^1/_4$ | | |
| O17 | 6*h* | *m*.. | 0.327 | 0.304 | $^1/_4$ | | single atom Mo |
| O18 | 6*h* | *m*.. | 0.353 | 0.159 | $^1/_4$ | | non-coplanar triangle $Mo_3$ |
| Mo19 | 6*h* | *m*.. | 0.4273 | 0.3042 | $^1/_4$ | | octahedron $O_6$ |
| P20 | 6*h* | *m*.. | 0.4574 | 0.0333 | $^1/_4$ | | tetrahedron $O_4$ |
| O21 | 6*h* | *m*.. | 0.553 | 0.294 | $^1/_4$ | | |
| O22 | 6*h* | *m*.. | 0.561 | 0.076 | $^1/_4$ | | non-colinear PMo |
| O23 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.099 | 0.5 | single atom P |
| P24 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.218 | 0.5 | |
| O25 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.579 | 0.5 | single atom Mo |
| Mo26 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.7055 | 0.5 | |
| $(OH_2)$27 | 4*e* | 3.. | 0 | 0 | 0.232 | 0.5 | |
| Cs28 | 2*b* | -3.. | 0 | 0 | 0 | 0.797 | colinear $(OH_2)_2$ |

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.054, T = 294 K

Remarks: Homogeneity range $Cs_{8+x}(MoO_4)Mo_{12}O_{18}(PO_4)_{10}\cdot H_2O$, $0 < x < 1$. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hoareau T., Leclaire A., Borel M.M., Grandin A., Raveau B. (1994), Eur. J. Solid State Inorg. Chem. 31, 727-737.