

Table M20-ii-001. KOH. Fractional coordinates and temperature parameters at 294 K [85Jac]. U_{ij} [$\cdot 10^{-3} \text{ \AA}^2$] is defined by Eq. (d) in Introduction.

KOH 294 K	
$x(\text{K})$	0.1718(2)
$y(\text{K})$	1/4
$z(\text{K})$	0.2876(1)
$x(\text{O})$	0.3194(6)
$y(\text{O})$	1/4
$z(\text{O})$	0.7699(5)
$U_{11}(\text{K})$	21.8(2)
$U_{22}(\text{K})$	19.9(2)
$U_{33}(\text{K})$	32.7(2)
$U_{12}(\text{K})$	0
$U_{13}(\text{K})$	8.5(2)
$U_{23}(\text{K})$	0
$U_{11}(\text{O})$	24.2(8)
$U_{22}(\text{O})$	26.3(9)
$U_{33}(\text{O})$	41(1)
$U_{12}(\text{O})$	0
$U_{13}(\text{O})$	5.8(8)
$U_{23}(\text{O})$	0

Table M20-ii-002. KOH. Fractional coordinates derived from neutron diffraction data [86Bas].

KOH at 293 K	
K at 2(e):	0.17, 1/4, 0.29
O at 2(e):	0.32, 1/4, 0.77
(1/2)H at 4(f):	0.46, 0.18, 0.90
KOH at 77 K	
K at 4(e):	0.44, 0.26, 0.29
O at 4(e):	0.28, 0.27, 0.78
H at 4(e):	0.27, 0.15, 0.92