

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

RbOH 294 K	
$x(\text{Rb})$	0.1623(7)
$y(\text{Rb})$	1/4
$z(\text{Rb})$	0.2843(6)
$x(\text{O})$	0.338(6)
$y(\text{O})$	1/4
$z(\text{O})$	0.778(5)
$U_{11}(\text{Rb})$	26.2(8)
$U_{22}(\text{Rb})$	14.5(7)
$U_{33}(\text{Rb})$	47(1)
$U_{12}(\text{Rb})$	0
$U_{13}(\text{Rb})$	14.0(7)
$U_{23}(\text{Rb})$	0
$U_{11}(\text{O})$	40(10)
$U_{22}(\text{O})$	9(6)
$U_{33}(\text{O})$	90(20)
$U_{12}(\text{O})$	0
$U_{13}(\text{O})$	20(10)
$U_{23}(\text{O})$	0