

M20 KOH group

Table M20-i-001. NaOD, NaOH. Fractional coordinates and temperature parameters [85Jac]. U_{ij} [$\cdot 10^{-3} \text{ \AA}^2$] and B [\AA^2] are defined, respectively, by Eq. (d) and Eq. (e) in Introduction.

	NaOH 294 K	NaOH 147 K	NaOD 298 K
$x(\text{Na})$	0	0	0
$y(\text{Na})$	0.3381(2)	0.3377(2)	0.3361
$z(\text{Na})$	1/4	1/4	1/4
$x(\text{O})$	0	0	0
$y(\text{O})$	0.1338(3)	0.1345(4)	0.1338
$z(\text{O})$	1/4	1/4	1/4
$x(\text{H})$	0	0	0
$y(\text{H})$	0.052(5)	0.055(7)	0.0532
$z(\text{H})$	1/4	1/4	1/4
$U_{11}(\text{Na})$	13.7(8)	1(1)	
$U_{22}(\text{Na})$	29(1)	13(1)	
$U_{33}(\text{Na})$	19.3(9)	12(1)	
$U_{12}(\text{Na})$	0	0	
$U_{13}(\text{Na})$	0	0	
$U_{23}(\text{Na})$	0	0	
$U_{11}(\text{O})$	15(1)	2(2)	
$U_{22}(\text{O})$	26(2)	12(2)	
$U_{33}(\text{O})$	20(2)	14(2)	
$U_{12}(\text{O})$	0	0	
$U_{13}(\text{O})$	0	0	
$U_{23}(\text{O})$	0	0	
$B(\text{H})$	3(2)	0(2)	

Table M20-i-002. NaOD, NaOH. Mean square displacements at $T = 578 \text{ K}$ [82Ble]. $\overline{u^2} = B/(8\pi^2)$; B is defined by Eq. (e) in Introduction.

NaOH	$\overline{u^2}$ [\AA^2]	NaOD	$\overline{u^2}$ [\AA^2]
Na	0.18(2)	Na	0.15(2)
O	0.09(1)	O	0.08(1)